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LIQUID CHROMATOGRAPHIC ANALYSIS OF NITROCELLULOSE-BASE PROPELLANTS: FINAL REPORT OF SECOND YEAR

James G. Carver
Propulsion Directorate
Research, Development and Engineering Center

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U.S. ARMY MISSILE COMMAND
Redstone Arsenal, Alabama 35898-5000

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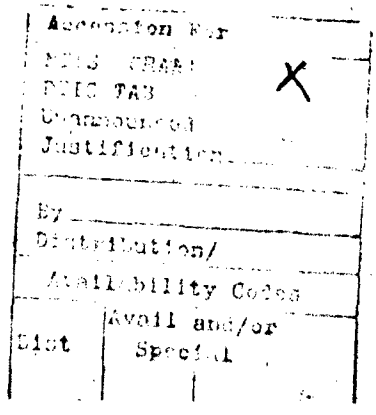

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A procedure has been developed that is able to predict the optimum conditions for separation of the ingredients of a complex mixture by liquid chromatography. The procedure involves establishing a data base of retention times for a large number of propellant ingredients in 7 predetermined combinations of 3 solvents. When a new combination of some of these ingredients is encountered, a computer analysis of the retention times of the ingredients from the data base will predict the best solvent composition to separate all the ingredients. The details of the procedure and several examples of its use are discussed.

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I. INTRODUCTION

Nitrocellulose-based propellants are widely used throughout the military and civilian areas in guns and rockets. There are almost as many different procedures for analysis as there are propellants. Even in the area of liquid chromatography, frequently, more than one procedure is used in the analysis of the propellant. Most techniques have been designed to answer a specific question about the purity or amount of two or three ingredients. However, most propellants have at least three or four original ingredients and frequently one or two other reaction products that can be easily extracted.

Since these ingredients can be extracted into a solvent it would seem logical to try to analyse for all of them at one time. Early efforts centered on developing separations using silica columns such as Corasil II and eluting with non polar solvents such as hexane, methylene chloride, and dioxane [1-14]. A major difficulty to this in the past has been that silica columns are difficult to work with. Precise control of water, alcohols, and other polar ingredients is necessary to obtain reproducible retention times and amounts.

II. BACKGROUND

Chromatographic efforts shifted to reverse phase separations with the advent of permanently bonded phases and improved equipment. Reverse phase columns do not have the problems that silica columns do. Materials are separated on differences in their nonpolar segments rather than in their polar segments as in silica columns. Currently over 80% of all HPLC separations are performed on reverse phase columns [15], but investigators have expressed difficulty in obtaining good separations of complex mixtures with the binary solvent mixtures commonly used [16-18]. Nonetheless, analysis times have been shortened from 10 to 12 hours using the older MIL-STD-286B methods to less than one hour using HPLC [19-20].

Recently, significant interest has been observed in using more than 2 solvent systems with C-18 columns. Manufacturers have started producing HPLC equipment that can pump 3 or 4 solvents simultaneously. The reason for a multi-solvent system is that separations are accomplished by more than differences in polarity. Snyder [21] has proposed that solvents should be classified as to three properties: proton acceptor, proton donor, and dipole interaction. It is believed that these properties make the major contributions to separations in HPLC. Kirkland [22] has developed a procedure consisting of 7 experiments which can be used to predict the best solvent composition for separating ingredients in a mixture. A program was undertaken to develop a procedure that will separate the maximum number of commonly used propellant ingredients possible.

Previously [23] a procedure was described where with a series of 7 experiments the separation of up to 10 propellant ingredients would be optimized. The procedure is not one that should be used for every unique analytical problem encountered but shows great promise for the occasionally difficult cases and for repetitive analysis. In production facilities this latter case will be of significant aid. Frequently, several samples of the same material require rapid analysis each day. It is not unusual for more than one formulation to be in production at the same facility. Isocratic separations are desired for their reproducibility and turn around time, also no column

reequilibration is required. If one set of conditions could be used for all the formulations manufactured at the facility, the samples could be analysed in a random or as received order rather than in groups.

At the time of writing the first paper on this subject several limitations still existed. The computer program employed could only work with 10 ingredients and was limited to a 64K mini computer operating in Basic. This limitation was imposed by computer memory restrictions. A disc based computer was recently made available to the RD&E Center laboratory. With the computers increased capabilities for large matrix operations it was possible to modify the program to consider many more materials simultaneously. A limit of 35 ingredients was arbitrarily selected as the maximum number for calculations. A program this size performs a complete evaluation to 595 pairs of ingredients. As a practical limit 20 propellant ingredients were selected for further work.

A new disc based program has now been written. It includes several improvements over the original program such as calculating with the actual peak widths rather than an average, and plotting all resolution lines on one graph on a x-y plotter. This program has been written in Basic. A Fortran 77 version is also available. See Appendix B for Basic programs "XLDB6 and XLDB6B", see Appendix C for Fortran 77 program "LC Main".

III. EXPERIMENTAL

The chromatographic system consisted of a Waters Associates 720 System Controller, 710B WISP sample injector, three M6000 pumps, a Perkin-Elmer LC 85 variable wavelength ultra violet detector and either a Supleco 250 mm x 4.6 mm ID Supelcosil 5 micron C-18 column or a Dupont 5 micron ZORBAX ODS 4.6 mm x 250 mm column. Solvents were from Burdick and Jackson and were filtered prior to mixing. Solvents in this study were combinations of the identified solvent and distilled deionized water. MeOH is 60% methanol-40% water, ACN is 50% acetonitrile-50% water, and THF is 42% tetrahydrofuran-50% water.

The analog UV signal was digitized and sent to a Hewlett-Packard 3357 Laboratory Automation System for data reduction. Following normal integration, a computer program was automatically run that calculated the peak widths and retention times required for input to the solvent selection program (see Basic program "Peak WT" in Appendix A).

Samples were prepared by cutting a propellant into small pieces and accurately weighing 50-100 mg into a 15 ml test tube. An accurately weighed internal standard was added to the test tube and then 10 ml of a 50% acetonitrile/water solution was added. An ultrasonic micro tip was placed in the test tube and the sample was extracted for 15 minutes. The solution was filtered and placed in a WISP sample vile for analysis.

A 50% acetonitrile solution was selected because noncross linked nitrocellulose samples will dissolve completely or form a gum in pure acetonitrile. If this solution is filtered or injected onto a column the nitrocellulose would plug the pores.

When HMX is suspected in the sample and quantitative analysis is required, a smaller sample or greater amount of solvent is needed. HMX has only a limited solubility in even pure acetonitrile. RDX is much more soluble than HMX and should not present a problem. You must allow for the presence of HMX and RDX even when no qualitative data is required, when selecting the optimum chromatographic solvent.

IV. SOLVENT SELECTION

A column is first characterized by determining the retention times and peak widths of all known propellant ingredients in 7 predetermined solvent compositions. This data is fed into a computer file for later reference. This only needs to be done once for each column (see Table 1). This procedure has been described earlier [22].

Most samples are submitted for analysis in RD&E Center laboratory as part of an aging surveillance program or for verification of composition. In these cases the computer is asked to analyse the data file for only those ingredients known or suspected to be present in the propellant extract. A typical example of this procedure is the N-5 propellant.

The frest propellant is known to contain Nitroglycerine, Diethylphthalate, and 2-Nitrodiphenylamine. The binder, lead salts, and other insoluble ingredients are not considered. As the propellant ages, degradation products of 2-NDPA are expected to be produced. Therefore, the computer was asked to predict the best conditions for separation of 2,2-Dinitro DPA, 2,4-Dinitro DPA, and 2,4,4-Trinitro DPA, an internal standard Dipropylphthalate, as well as the three original ingredients. It predicted the best solvent composition for the separation would be 82% MeOH/18% ACN with a minimum resolution of 2.855 for any two peaks (see Table 2). The triangular graph (Figure 1) indicated good resolution could be obtained with MEOH/ACN combinations between 86/14 and 78/22. Since methanol has a higher viscosity than acetonitrile the 78/22 mixture was selected. This permitted a higher flow rate than possible with the 82/18 mixture.

As can be seen in the chromatograph of the standard sample (Figure 2), all the ingredients were well resolved with the 78/22 mixture at 2.0 ml/min. Once the system was calibrated the propellant samples were analysed.

V. DISCUSSION

One aspect of the procedure that has been receiving attention is its ability to predict optimized conditions for any combination of ingredients in a data base. Once the retention times of a large number of ingredients have been determined for the 7 solvent compositions, the optimum conditions for any combination of those ingredients can quickly be predicted without further experimentation. A drawback to this is the data base for a Waters 10 micrometer C-18 radial pack is not necessarily comparible to another column such as a Waters 10 micrometer steel column. To explore how significant column differences effected the predicted optimum conditions a data base was established for several different columns. Tables 3 thru 7 list the retention times for 20 propellant ingredients in the 7 solvent compositions. As reported earlier, MeOH signifies 60% methanol in water, ACN signifies 50% acetonitrile in water, and THF signifies 42% tetrahydrofuran in water. Table 8 lists the important

specifications for the 5 columns tested. Three Waters 10 micrometer C-18 Radial Pac columns were tested. The computer predicted almost exactly the same optimum conditions for all three. The obvious implication is that for these bulk loaded columns the column to column reproducibility is very good. It should be noted however that this data was obtained using a RCM-100 modual. The Z-modual uses slightly different columns and produce different results even though they have the same name.

Following the procedure described earlier, the computer predicted optimum solvent compositions were determined for each of the 5 different columns. As seen in Figure 3 most of the columns have a optimum composition in the same general area.

Not unexpectedly, a significant improvement in resolution was obtained in changing from a 10 micrometer packing to a 5 micrometer packing. Figure 4 is a chromatographic run using a 5 micrometer Waters C-18 Radial Pac column at the optimum solvent composition. Figure 5 is a run of the same solvent but on a 10 micrometer C-18 Radial Pac column.

Eighteen ingredients can be separated well enough to quantify at the predicted composition for the 5 micrometer Waters column (Figure 4). Two pairs of these peaks appear as fused peaks while the remaining ingredients are well resolved. Only ethylcentralite and diphenylamine are unresolved at this composition. In Figure 5, the 10 micrometer Waters column shows almost no completely resolved peaks for the same conditions.

At the predicted optimized conditions for the Perkin-Elmer HS-5 C-18 column we see that several of the later peaks have shifted (Figure 6). Nitroglycerine has fused with 2,4 DNT and ethylcentralite with TNT. Diphenylamine has eluted later and is almost resolved completely from BTTN. Four pairs are completely unresolved: resorcinol and triacetin; RDX and methylcentralite; 2,4 DNT and nitroglycerine; TNT and ethylcentralite. Generally the ingredients appear to be less resolved than in the Waters 5 micrometer radial pac system.

A suplecosil LC-18 column (Figure 7) was optimized for separating the mixture. Again the predicted solvent composition was similar to the previous examples. Comparison with the Perkin-Elmer column shows that ethylcentralite and TMETN have shifted relative to the other ingedients. Diphenylamine is completely resolved as is TNT but now the ethylcentralite is co-eluting with BTTN. The resolution of fused peaks is better than in the Perkin-Elmer column but there are still 4 pairs of co-eluting peaks.

The Dupont Zorbax ODS column had a predicted optimum significantly different from the others. Figure 8 indicates complete resoltuion of all the ingredients. Dupont literature discusses the unique properties of their Zorbax columns. They are manufactured with monofunctional silane units to produce a "monolayer". Whether or not the characteristics of this column are unique or common to all Zorbax ODS columns will have to be determined. The long elution times of the last 4 ingredients is undesirable but if the analyst wishes to use an isocratic system this situation is unavoidable. A change in the solvent composition after 17 minutes could cause these ingredients to elute faster with minimal loss of resolution. This would introduce an equilibration delay between runs however, so a trade off would have to be

made. Using the solvent composition chosen for the Supelco column, this Dupont column produced a chromatogram similar to Figure 7 except that nitroglycerine and ethylcentralite appear as fused peaks to 2,4 DNT and BTTN respectively.

Figure 9 represents a chromatogram of the Waters 10 micrometer Radial Pac column at its best composition near the selected Dupont composition. There is some shifting of peaks but the chromatograms appear similar. The most important difference is the significant loss of resolution. There are 4 fused peak pairs and 4 sets of unresolved peaks. While on first glance Figure 9 appears to be better than Figure 4, close examination indicates more partially resolved ingredients than in Figure 9. So the original predicted optimum composition for the Waters column is indeed better than the alternate.

VI. ANALYSIS OF UNKNOWN

Occasionally, a propellant of unknown composition is submitted for analysis. A variety of analytical tools are employed for this task.

For LC analysis, the solvent capable of separating, at least partially, all known ingredients is initially selected. Retention times of the unknown peaks are compared with the predicted retention times. The retention times of the authentic ingredients are then obtained for comparison. Once a list of probable ingredients is obtained, the computer selects a second solvent to separate these specific materials. Standards are then prepared and the analysis proceeds normally.

One foreign propellant (#1) analysed in this laboratory was found to be a rather simple double-base composition. The extractables were identified as nitroglycerine, NDPA, and methylcentralite. Excellent resolution was easily obtained with 100% MeOH.

A second foreign propellant (#2) provided a greater challenge. After some work it was found to contain DEGDN, methylcentralite, 2,6-DNT, 2,4-DNT, 2,4,6-TNT, nitroglycerine, NDPA, and DPA. An internal standard of Dipropylphthalate was selected. A solvent composition of 60% MeOH-40% THF was chosen. Figure 10 shows the resulting chromatogram.

A third foreign propellant (#3) turned out to be a single base nitrocellulose propellant stabilized with diphenylamine (Figure 11). The interesting point is that the propellant appears to be contaminated with trace amounts of HMX, RDX, MNA, TMETN, 4-NDPA, and 2-NDPA. NDPA was also found but it is probably a degradation product from the DPA. Blanks were prepared and the contamination was only found in the propellant extract. It was concluded that the manufacturing facility was also engaged in production of other more sophisticated propellants.

VII. COMPARISON OF TECHNIQUES

Since the analysis of propellants has a greater confidence level when similar values are obtained by two different procedures, GC analyses of several propellants were obtained for comparison with the LC data.

N-5 samples aged in tropic, arctic, or desert conditions were examined by capillary GC for 2-NDPA to determine their remaining shelf life. LC analysis of the samples included nitroglycerine, diethylphthalate, 2,2-Dinitro DPA, and 2,4-Dinitro DPA as well as 2-NDPA. The results indicate good agreement for the two techniques (Table 9). As seen in the table and chromatograms (Figures 12, and 13), formation of the 2-NDPA degradation products proceeded further in the hotter temperature conditions and agrees with the decrease of 2-NDPA. A potential method for an internal check is to compare the total amount of 2-NDPA and its products with the initial amount of 2-NDPA in the propellant. The millimolar ratios of 2,4-Dinitro DPA and 2,2-Dinitro DPA are identical at 2.62 for the desert and tropic samples. The millimolar amounts of 2-NDPA and its products are the same for the arctic and tropic at 8.37 and 8.43, respectively. The desert is out of line with 9.29 millimoles per 100 μg of propellant. A time zero analysis for this lot is not available; therefore, it is difficult to determine whether the discrepancy is due to a greater amount in the initial propellant or an error in the analysis. As pointed out above, the molar ratios of dinitro products are the same for desert or tropic and the total amount of 2-NDPA and dinitro products is the same for arctic or tropic. Therefore, the most likely explanation is a different amount of initial 2-NDPA.

CHAPARRAL propellant has been examined by both GC and LC techniques in RD&E Center laboratory. Several aged motors of different production lots were analysed to determine residual levels of MNA, 2-NDPA, and 4-NDPA. Additionally, the levels of nitroglycerine, BTTN and nitroso MNA were determined. Table 10 presents a summary of the results. Generally, the two procedures agree within a few percent of each other for MNA and n-MNA, but there are a few cases where as much as 9% disagreement was observed. The cause of this is not immediately clear. The total molar amounts of MNA and n-MNA as determined by the two techniques do not show a pattern other than that when aged hot the LC sees less material in the propellant than the GC and when aged at ambient the LC see more material than the GC. This may be caused by the incomplete separation of MNA and HMX. Further study will be needed to answer this question.

The SPRINT propellant is a composite modified double-base propellant. Analysis was performed for nitroglycerine, 2-NDPA, triacetin, resorcinol, and 2-nitroresorcinol. The latter was not separated by GC and the different response factors may be responsible for the different values in LC and GC. The triacetin does not absorb strongly in the UV and while resolved fairly well small fluctuations in the base line or near by peaks could significantly alter the calculated value (Figure 14). Generally, however, there is good agreement between the two techniques (Table 11).

Two foreign propellants were analysed by HPLC and capillary GC. The analyses are given in Tables 12 and 13. As mentioned earlier, GC is not able to resolve some nitroderivatives from their parent compounds where LC can. Here NDPA and DPA present such a situation. In Foreign Propellant #1, GC found 0.15% DPA while LC found no DPA and 0.40% nitroso DPA. In Foreign Propellant #2, GC found 0.47% DPA while LC found 0.36% DPA and 0.25% NDPA which corresponds, after correcting for molecular weight differences, to 0.57% DPA in the initial propellant. Again, there is otherwise generally good agreement between the LC and GC techniques.

M-36 propellant points out one of the important limitations of LC. Even if it can be separated, measurement is impossible if it is not visible. Currently, liquid chromatography has only a few detection methods available. UV is the most popular, but many compounds of interest do not absorb well so they are detected poorly. Dipropyladipate is one such compound and as discussed above triacetin is another. The chromatogram in Figure 15 indicates that dipropyladipate can indeed be well resolved from the other ingredients in M-36 propellant. Table 14 indicates that while several GC techniques using flame ionization detectors obtained an average value of 3.02% di-n-propyladipate with 0.5% relative standard deviation, LC came up with 4.04%. This is more than a 33% difference between techniques. It is hoped that newer LC detectors such as electrochemical or micro LC/Flame detectors can solve this problem.

VIII. UNIVERSAL PROCEDURE

No truly universal procedure exists. In a production facility such as Radford AAP several different formulations are being manufactured simultaneously. These formulations are chemically different only in the amount of a limited number of ingredients. Typically several solvent compositions would be required for HPLC analysis of these formulations. It is very probable that with the above described procedure one solvent composition could be quickly selected that would be able to separate all the materials in all the formulations. Thus, samples could be analysed as received or in a random order rather than holding a sample until a group using the same solvent is assembled. As an example of this, a solvent was selected that could separate 20 of the most commonly used propellant ingredients (see Figure 7). It is clear that only one set of conditions is needed to quantify any combination of these materials.

IX. CONCLUSIONS

The procedure described here seems to have almost universal application in liquid chromatography. Once the retention times for a list of ingredients is developed no further experimentation is required. When a new propellant composition is encountered, the solvent composition necessary for optimum separation of the ingredients can be quickly predicted with the aid of a computer.

The best separation achieved to date was with a 5 micrometer spherical particle coated with a "monolayer" of C-18. Other columns of this type need to be evaluated to determine column to column reproducibility. The computer program can evaluate up to 35 double base ingredients but with the columns evaluated to date a practical limit is 20 ingredients per sample. This may be improved by using 3 micrometer columns. Employing a second selective detector such as a fluorescence or an electrochemical detector should offer the better solution however.

In a production situation this procedure can quickly predict a single solvent composition that can separate up to 20 ingredients. This should permit the analysis of all the different formulations manufactured at a facility with one set of conditions resulting in a more complete analysis and more rapid turn around time in situations presently requiring several sets of conditions or gradient elutions.

It has been demonstrated that when a new formulation of known composition is encountered, an optimum solvent composition can be predicted without experimentation once a column has been characterized. It is recommended that when a column is replaced with a similar column from the same manufacturer, the column should be tested at the optimum solvent composition for the first column. If no significant differences are observed then the same data base can be used as before. Columns from different manufacturers will probably have different characteristics and should be completely characterized routinely.

Clearly, a procedure exists that can quickly obtain good separations of the extractable ingredients from a double-base or composite modified double-base propellant. LC is capable of resolving some materials and their degradation products that GC can not. Comparison of GC and LC analyses of several propellants indicates that the two techniques give approximately the same results for those ingredients that they can both detect. LC is superior to GC in its ability to separate certain materials and to detect many nonvolatile materials, such as HMX. GC is superior to LC for detection of some materials. LC and GC techniques thus appear to complement each others weaknesses and strengthen the validity of the propellant analysis. Therefore, it is recommended both techniques be used for critical determinations. Otherwise, the analyst should determine what he wants from the analysis and select the appropriate technique.

Table 1. HPLC Optimization.

INPUT DATA
COLUMN : SUPLECO 5u C-18 SAMPLE : GENERAL
DATA IS CORRECTED TO 1.00 ml/min
PEAK WIDTHS IN SECONDS IN PARENTHESES

		MEOH 1	ACN 2	THF 3	ACN& MEOH 4	THF& MEOH 5	ACN& THF 6	MEOH& ACN&THF 7
	Solvent Front	1.78	1.79	1.79	1.78	1.79	1.79	1.79
1	Resorcinol	3.17	3.08	3.88	3.24	3.51	3.45	3.41
		(14)	(12)	(12)	(12)	(12)	(12)	(12)
2	HMX	3.17	5.14	5.61	4.25	5.76	4.68	4.72
		(14)	(17)	(14)	(13)	(14)	(13)	(13)
3	RDX	4.07	5.14	6.19	4.95	7.28	5.19	5.63
		(25)	(23)	(17)	(13)	(17)	(14)	(14)
4	DEGDN	4.64	6.52	7.81	5.93	7.63	6.16	6.26
		(18)	(33)	(18)	(14)	(18)	(15)	(15)
5	MNA	5.14	5.82	5.83	5.95	6.26	5.46	5.75
		(19)	(18)	(15)	(15)	(15)	(14)	(14)
6	Nitroglycerine	6.49	9.08	16.03	8.50	16.07	10.15	10.73
		(12)	(26)	(44)	(20)	(44)	(22)	(22)
7	Acaradite I	5.96	4.49	3.65	6.02	4.25	3.90	14.53
		(24)	(21)	(12)	(15)	(14)	(12)	(44)
8	2,4,6 TNT	6.91	9.25	24.06	9.18	15.59	10.80	11.24
		(24)	(26)	(64)	(20)	(44)	(28)	(39)
9	BTTN	6.95	10.21	16.17	9.66	17.23	10.69	11.97
		(25)	(28)	(44)	(22)	(50)	(28)	(39)
10	2,6 DNT	7.65	8.70	11.63	9.51	11.83	8.46	9.47
		(35)	(23)	(39)	(21)	(39)	(20)	(21)
11	Acaradite II	6.86	5.21	4.00	7.21	5.65	4.43	5.07
		(27)	(20)	(13)	(18)	(14)	(14)	(14)
12	TMETN	9.28	12.81	25.44	12.82	24.49	14.05	16.01
		(46)	(34)	(65)	(38)	(64)	(39)	(40)
13	NDPA	19.96	18.61	17.42	24.62	26.50	16.95	23.04
		(49)	(40)	(44)	(64)	(64)	(40)	(58)
14	4 NDPA	17.86	15.07	14.84	21.09	22.06	13.72	18.81
		(44)	(40)	(40)	(53)	(55)	(39)	(50)
15	Meth Centralite	14.64	9.39	6.51	15.32	8.04	7.01	8.69
		(52)	(36)	(17)	(40)	(20)	(17)	(22)
16	DPA	36.63	19.36	11.13	38.97	16.29	12.35	18.17
		(55)	(44)	(39)	(60)	(38)	(35)	(40)
17	2 NDPA	35.06	24.40	18.75	37.27	30.74	19.32	26.91
		(104)	(64)	(40)	(60)	(55)	(52)	(68)
18	Ethyl Centralite	14.89	15.54	6.48	19.39	14.59	11.55	14.20
		(117)	(79)	(15)	(55)	(40)	(39)	(40)
19	Triacetin	3.88	4.17	3.61	4.54	4.05	3.73	3.90
		(19)	(27)	(49)	(15)	(40)	(29)	(33)
20	Tetryl	4.28	5.24	6.13	5.29	7.99	5.24	5.95
		(21)	(22)	(26)	(83)	(84)	(23)	(26)
21	TEGDN	5.02	7.14	7.44	6.62	7.64	5.99	6.40
		(31)	(21)	(23)	(29)	(25)	(19)	(21)
22	Nitroso-MNA	6.11	7.23	8.31	7.62	8.64	6.59	7.26
		(27)	(20)	(27)	(21)	(26)	(20)	(23)
23	2 N-Resorcinal	3.83	4.20	4.89	4.35	5.17	4.45	4.63
		(21)	(14)	(16)	(15)	(19)	(15)	(16)
24	2,4 DN Resorcin	1.89	1.84	1.84	2.00	2.19	1.89	2.03
		(16)	(16)	(20)	(15)	(24)	(16)	(20)
25	2,4 DNT	8.07	8.68	11.61	9.68	13.20	8.57	10.04
		(33)	(21)	(32)	(26)	(36)	(24)	(28)
26	2,4,4 TN DPA	13.78	15.39	10.02	20.82	29.28	16.43	20.13
		(56)	(42)	(80)	(60)	(75)	(54)	(62)
27	2,4 DN DPA	17.21	16.53	19.20	22.75	23.58	14.92	19.14
		(55)	(44)	(51)	(65)	(70)	(68)	(92)
28	2,2 DN DPA	21.60	18.03	12.66	26.46	24.19	14.08	19.82
		(83)	(27)	(37)	(73)	(71)	(41)	(57)
29	Methylphthalate	5.44	5.85	4.62	6.64	5.33	4.84	5.22
		(25)	(17)	(23)	(21)	(19)	(24)	(13)
30	Ethyl Phthalate	9.72	9.82	6.85	12.41	8.21	7.29	8.35
		(42)	(27)	(22)	(37)	(94)	(23)	(115)
31	Propylphthalate	24.38	21.52	12.36	32.20	17.49	13.82	18.07
		(93)	(58)	(36)	(91)	(56)	(41)	(53)

Table 2. HPLC Optimization.

9:00 AM TUE., 14 AUGUST 1984

DATA ANALYSIS
COLUMN: SUPELCO 5u C-18 SAMPLE: N-5 PROPELLANT

THE BEST COMPOSITION IS:

MEOH	ACN	THF
82%	18%	0%

THE WORST RESOLUTION AT THIS POINT IS 2.655

PREDICTED ORDER OF ELUTION

INGREDIENT	RELATIVE RETENTION TIME 1.00 ml/min	1.50 ml/min
Nitrogylcerine	7.38	4.92
Ethyl Phthalate	11.30	7.54
2,4,4 TN DPA	17.76	11.84
2,4 DN DPA	20.57	13.71
2,2 DN DPA	24.89	16.59
Propylphthalate	29.34	19.56
2 NDPA	37.61	25.07

Table 3. Optimization of 5 Micron Waters C-18 Radial PAC.

	MEOH	ACN	THF	MEOH/ACN	MEOH/THF	ACN/THF	MEOH/ACN/THF
TRIACETIN	1.60	3.21	6.80	1.62	7.03	1.89	4.89
RESORCINOL	1.81	3.66	6.90	1.91	7.34	2.10	5.05
HMX	1.95	3.32	3.77	2.82	4.34	3.17	3.34
RDX	2.86	3.41	4.33	3.31	6.13	3.70	4.25
DEGDN	3.40	4.51	5.96	4.13	6.19	4.56	4.77
MNA	4.12	4.23	4.30	4.51	5.39	4.15	4.66
NG	4.35	6.36	14.45	5.69	12.86	8.12	9.05
ACARADITE I	4.74	3.20	2.33	4.40	3.15	2.70	3.27
TNT	4.85	6.42	21.72	6.16	13.30	8.78	9.00
BTTN	4.88	7.12	13.40	6.65	15.66	8.53	9.77
2,6 DNT	5.98	6.26	9.70	6.58	9.96	7.20	8.28
ACARADITE II	6.19	4.11	2.66	5.55	3.62	3.21	3.85
TMETN	6.45	9.00	22.05	8.88	22.09	11.41	13.28
2,4 DNT	6.93	6.36	9.65	7.03	10.50	7.12	8.41
EC	12.15	11.21	10.10	13.30	12.98	10.51	13.45
MC	13.14	8.09	5.03	12.02	6.60	5.63	7.87
4 NDPA	13.70	11.22	12.45	15.81	23.00	11.88	17.28
NDPA	13.96	12.98	15.95	15.78	23.50	15.50	21.60
2 NDPA	29.60	17.81	17.30	26.70	28.45	17.52	27.15
DPA	31.30	16.40	10.15	27.88	14.85	11.40	17.98

Table 4. Optimization of 10 Micron Waters C-18 Radial PAC.

	MEOH	ACN	THF	MEOH/ACN	MEOH/THF	ACN/THF	MEOH/ACN/THF
TRIACETIN	.93	1.16	1.59	1.38	1.00	1.38	1.50
RESORCINOL	.86	.80	1.05	.90	1.03	.93	.93
HMX	.93	1.40	1.57	1.40	1.87	1.37	1.51
RDX	1.40	1.53	1.82	1.69	2.49	1.57	1.66
DEGDN	1.75	2.01	2.52	2.13	2.71	1.99	2.30
MNA	2.10	1.83	1.82	2.34	2.30	1.80	2.10
NG	2.27	2.86	1.17	3.06	5.92	3.38	3.95
ACARADITE I	2.48	1.45	1.01	2.30	1.37	1.16	1.45
TNT	2.54	2.94	9.05	3.38	6.06	3.76	4.06
BTTN	2.57	3.20	5.11	3.71	6.61	3.68	4.43
2,6 DNT	3.17	2.80	4.09	3.53	4.46	2.91	3.49
ACARADITE II	3.36	1.99	1.15	3.02	1.57	1.37	1.71
TMETN	3.54	4.06	17.58	5.02	9.66	5.00	6.18
2,4 DNT	6.93	6.36	9.65	7.03	10.50	7.12	8.41
EC	19.56	7.65	4.08	16.51	6.51	4.50	7.15
MC	7.85	3.68	2.11	6.66	2.98	2.35	3.24
4 NDPA	7.59	5.12	5.74	8.97	9.17	5.17	7.48
NDPA	7.09	5.13	6.41	7.68	5.78	4.17	5.54
2 NDPA	18.17	8.24	7.11	15.37	12.91	7.18	11.22
DPA	7.88	5.93	6.41	9.08	10.34	6.14	8.75

Table 5. Optimization of 5 Micron Perkin-Elmer HS-5 C-18 Column.

	MEOH	ACN	THF	MEOH/ACN	MEOH/THF	ACN/THF	MEOH/ACN/THF
TRIACETIN	2.27	2.31	2.96	2.43	2.99	2.75	2.68
RESORCINOL	2.27	2.31	2.96	2.43	2.99	2.75	2.68
HMX	2.54	4.21	5.63	3.58	5.22	4.28	4.09
RDX	3.37	4.51	6.34	4.15	6.75	4.78	4.84
DEGDN	3.85	5.47	8.04	4.89	6.84	5.63	5.42
MNA	4.53	5.07	5.84	5.14	5.91	4.96	5.09
NG	5.14	8.18	17.00	6.91	14.51	9.92	9.78
ACARADITE I	4.94	3.48	3.13	4.69	3.72	3.34	3.69
TNT	5.42	8.27	29.00	7.24	14.44	10.42	9.43
BTTN	5.56	9.22	18.75	8.33	16.83	10.43	10.60
2,6 DNT	6.27	7.69	12.26	7.65	10.69	8.03	8.36
ACARADITE II	6.12	4.38	3.57	5.79	4.19	3.92	4.34
TMETN	7.46	11.02	30.00	10.77	23.21	13.84	14.40
2,4 DNT	6.58	7.63	11.88	7.51	10.79	8.11	8.29
EC	12.70	12.94	11.86	14.83	13.59	11.14	12.56
MC	13.31	8.18	6.40	11.93	7.69	6.63	7.89
4 NDPA	14.55	12.75	17.34	17.06	22.20	13.33	16.65
NDPA	14.94	14.93	19.26	17.56	38.23	15.91	19.35
2 NDPA	27.86	18.96	20.99	26.54	28.22	18.05	23.17
DPA	34.23	15.75	11.86	29.06	16.02	11.96	16.30

Table 6. Optimization of 5 Micron Supelcosil LC-18 Column.

	MEOH	ACN	THF	MEOH/ACN	MEOH/THF	ACN/THF	MEOH/ACN/THF
TRIACETIN	3.17	3.08	3.88	3.24	3.51	3.45	3.41
RESORCINOL	3.17	3.08	3.88	3.24	3.51	3.45	3.41
HMX	3.17	5.14	5.61	4.25	5.76	4.68	4.72
RDX	4.07	5.14	6.19	4.95	7.28	5.19	5.63
DEGDN	4.64	6.52	7.81	5.93	7.63	6.16	6.26
MNA	5.14	5.82	5.83	5.95	6.26	5.46	5.75
NG	6.49	8.08	16.03	8.50	16.07	10.15	10.73
ACARADITE I	5.96	4.49	3.65	6.02	4.25	3.90	14.53
TNT	6.91	9.25	24.06	9.18	15.59	10.80	11.24
BTTN	6.95	10.21	16.17	9.66	17.22	10.69	11.97
2,6 DNT	7.65	8.70	11.63	9.51	11.83	8.46	9.47
ACARADITE II	6.86	5.21	4.08	7.21	4.65	4.43	5.07
TMETN	9.28	12.81	25.44	12.82	24.49	14.05	16.01
2,4 DNT	8.03	8.71	11.45	9.47	12.08	8.75	9.38
EC	14.89	15.54	6.48	19.39	14.59	11.55	14.20
MC	14.64	9.39	6.51	15.32	8.04	7.01	8.69
4 NDPA	17.86	15.07	14.84	21.09	22.06	13.72	18.81
NDPA	19.96	18.61	17.42	24.62	26.50	16.95	23.04
2 NDPA	35.06	24.40	18.75	37.27	30.74	19.32	26.91
DPA	36.63	19.36	11.13	38.97	16.29	12.35	18.17

Table 7. Optimization of 5 Micron Dupont Zorbax ODS Column.

	MEOH	ACN	THF	MEOH/ACN	MEOH/THF	ACN/THF	MEOH/ACN/THF
TRIACETIN	3.06	2.88	3.53	3.30	3.50	3.42	3.49
RESORCINOL	3.06	2.88	3.53	3.30	3.50	3.42	3.49
HMX	3.23	5.22	5.48	4.55	5.88	4.88	5.17
RDX	5.20	5.56	6.23	5.64	8.69	5.53	6.39
DEGDN	6.19	7.11	8.01	7.33	8.74	7.07	7.49
NNA	7.33	6.56	6.09	7.74	7.47	6.31	6.88
NG	8.49	10.47	20.13	10.38	22.24	12.43	13.82
ACARADITE I	9.07	5.56	3.52	7.87	4.60	4.06	4.88
TNT	9.67	10.95	29.80	11.64	21.79	13.83	14.75
BTTN	9.74	11.57	19.77	12.04	23.28	13.45	15.43
2,6 DNT	11.83	10.53	13.21	12.14	16.39	10.05	12.35
ACARADITE II	11.53	7.11	3.968	10.03	5.19	4.72	5.65
TMETN	13.31	14.96	30.50	16.90	32.26	18.30	21.60
2,4 DNT	14.15	10.81	13.82	13.12	17.47	10.84	12.62
EC	27.12	20.46	12.32	26.95	20.71	14.31	19.17
MC	31.35	16.11	7.09	25.62	10.28	8.05	10.95
4 NDPA	28.48	18.76	17.76	30.00	31.00	18.27	25.32
NDPA	31.92	24.68	20.52	33.35	39.17	21.98	31.97
2 NDPA	73.83	34840	24.98	59.77	48.35	27.47	40.31
DPA	70.04	34.61	12323	62.94	22.35	15.31	24.15

Table 8. Column Specifications.

Source	Dimensions (MM)	Packing	Partical	Plates
Waters	100 x 5	u-Bondapac C-18	10 Micron Spherical	>5,000
Waters	100 x 5	u-Bondapac C-18	5 Micron Spherical	>9,000
Supelco	250 x 4.6	Supelcosil LC-18	5 Micron Spherical	20,614
E Merck	250 x 4.6	LiChrosorb RP-18	5 Micron Irregular	15,516
Dupont	250 x 4.6	Zorbax ODS	5 Micron Spherical	27,135
PERKIN-ELMER	125 x 4.6	P-E HS-5 C-18	5 Micron Spherical	>8,000

Table 9. N-5 Propellant Analysis.

	NG	DEP	2,2-DN DPA	2,4-DN DPA	LC 2-NDPA	GC 2-NDPA
Arctic	35.74	10.72	--	--	1.792	1.811
Tropic	35.88	10.88	0.090	0.236	1.534	1.716
Desert	35.91	11.13	0.201	0.526	1.388	1.379

Table 10. CHAPARRAL Propellant Analysis.

Comparison of Capillary GC and HPLC

Lot	Condition Aged	Analytical Method	MNA	N-MNA	2-NDPA	4-NDPA	NG	BTTN
E0001	Hot	GC	0.259	0.490	0.244	0.197	12.56	12.86
	Hot	LC	0.263	0.384	0.245	0.209	13.43	12.23
E0003	Ambient	GC	0.564	0.048	0.260	0.229	13.18	13.55
	Ambient	LC	0.609	0.033	0.257	0.230	13.14	13.45
E0003	Hot	GC	0.346	0.380	0.255	0.223	13.04	13.26
	Hot	LC	0.366	0.281	0.244	0.216	13.51	13.62
E0005	Ambient	GC	0.588	0.048	0.260	0.248	12.76	12.79
	Ambient	LC	0.622	0.029	0.256	0.256	12.84	12.74
E0005	Hot	GC	0.112	0.727	0.241	0.211	12.38	14.80
	Hot	LC	0.107	0.624	0.235	0.204	13.00	14.99
E0006	Ambient	GC	0.569	0.042	0.251	0.222	12.81	14.57
	Ambient	LC	0.623	0.022	0.239	0.220	12.75	14.45
E0007	Ambient	GC	0.597	0.039	0.260	0.250	12.95	12.97
	Ambient	LC	0.637	0.024	0.247	0.249	12.80	12.78
E0008	Ambient	GC	0.626	0.023	0.261	0.254	13.26	12.64
	Ambient	LC	0.682	0.022	0.254	0.250	12.94	12.46
E0008	Hot	GC	0.205	0.644	0.340	0.218	13.03	13.65
	Hot	LC	0.218	0.530	0.323	0.210	13.41	13.73
GCU	Ambient	GC	0.615	0.115	0.256	0.261	13.28	14.13
	Ambient	LC	0.659	0.061	0.248	0.239	13.66	14.34

Table 11. Sprint Propellant Analysis.

	Triacetin	Resorcinol	2-Nitrorescinol	NG	2-NDPA
LC	6.657	0.950	0.019	28.734	0.942
GC	6.325	0.901	--	28.400	0.966

Table 12. Foreign Propellant #1 Analysis.

	NG	DPA	MC	NDPA
GC	39.25	0.153	1.104	--
LC	39.41	--	1.345	0.404

Table 13. Foreign Propellant #2 Analysis.

	DEGDN	NG	2,6 DNT + 2,4 DNT	2,4,6 TNT	MC	DPA	NDPA
LC	14.22	17.75	(0.905)	0.375	2.516	0.361	0.249
GC	14.64	17.41	(0.918)	0.356	2.550	0.474	--

Table 14. M-36 Propellant Analysis.

		NG	DNDPA	2-NDPN
GC	Splitless	39.151	3.017	1.950
GC	On-Column	39.134	3.046	1.961
GC	Manual/Split	39.117	3.011	1.969
GC	Auto/Split	39.182	3.002	1.962
GC	Auto/Split	39.012	3.016	1.954
LC		38.626	4.040	1.777

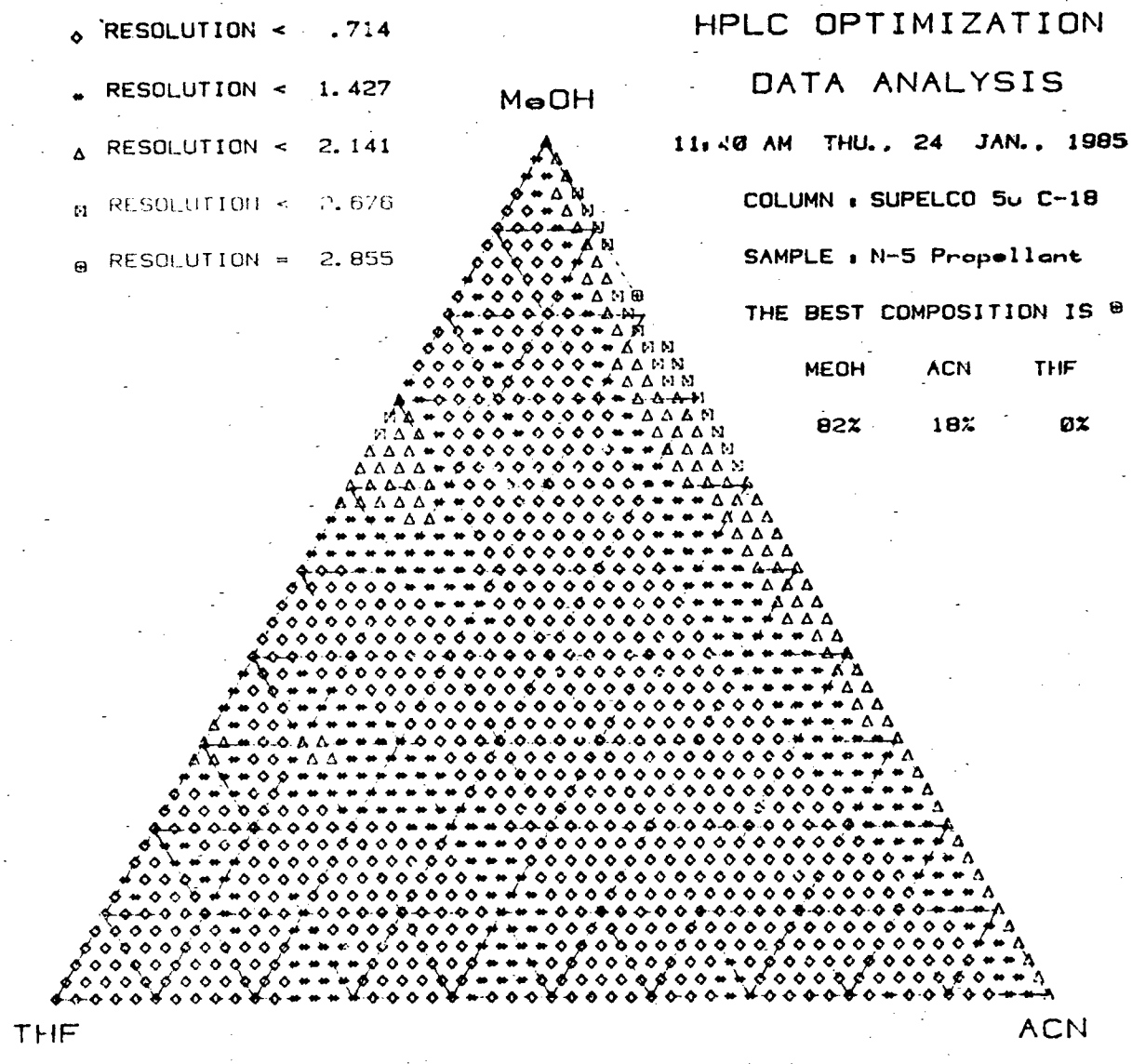

Figure 1. HPLC optimization data analysis.

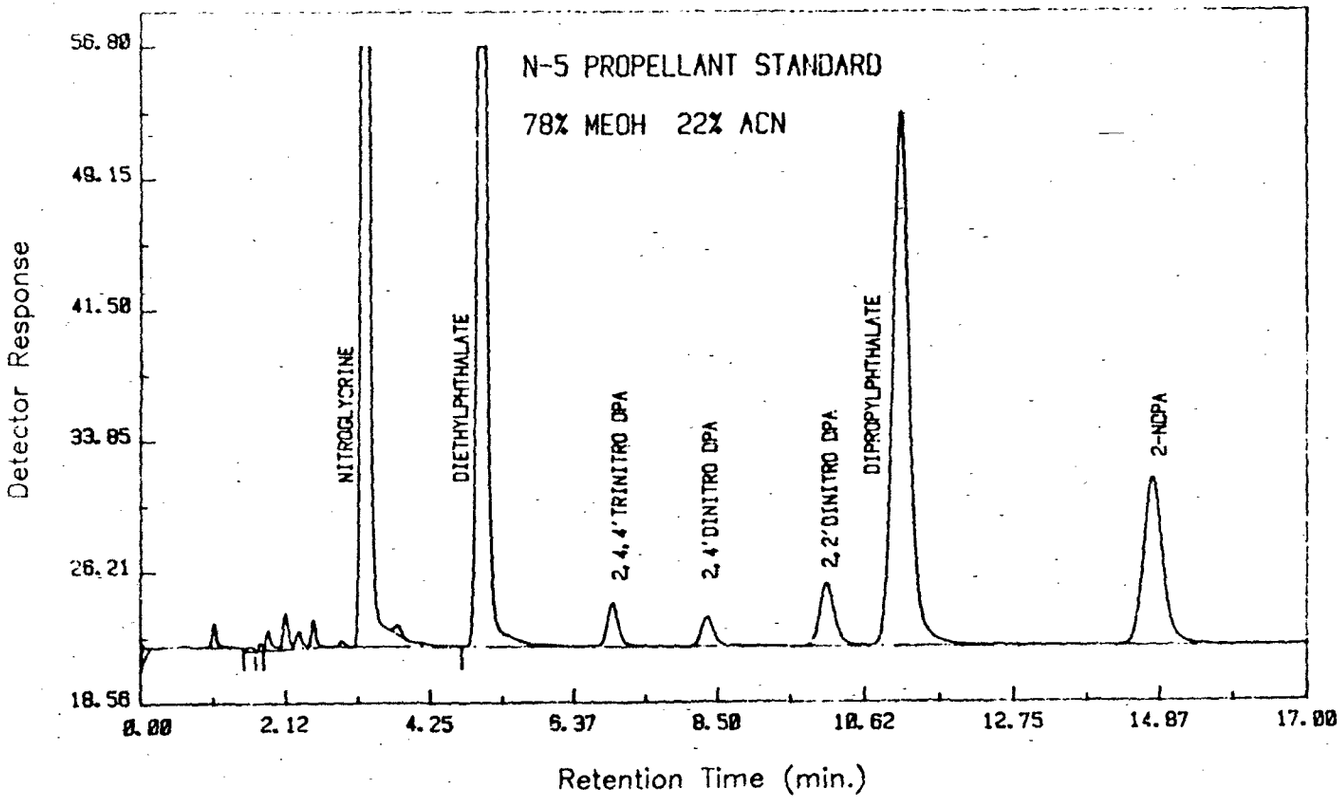

Figure 2. Standard sample.

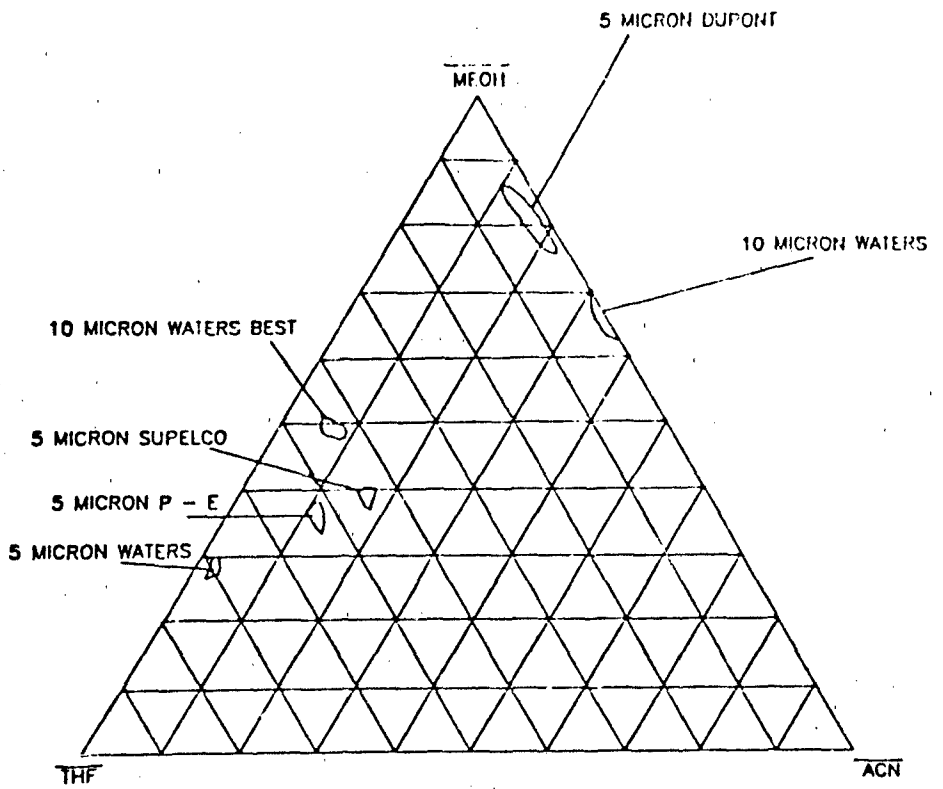

Figure 3. Column composition.

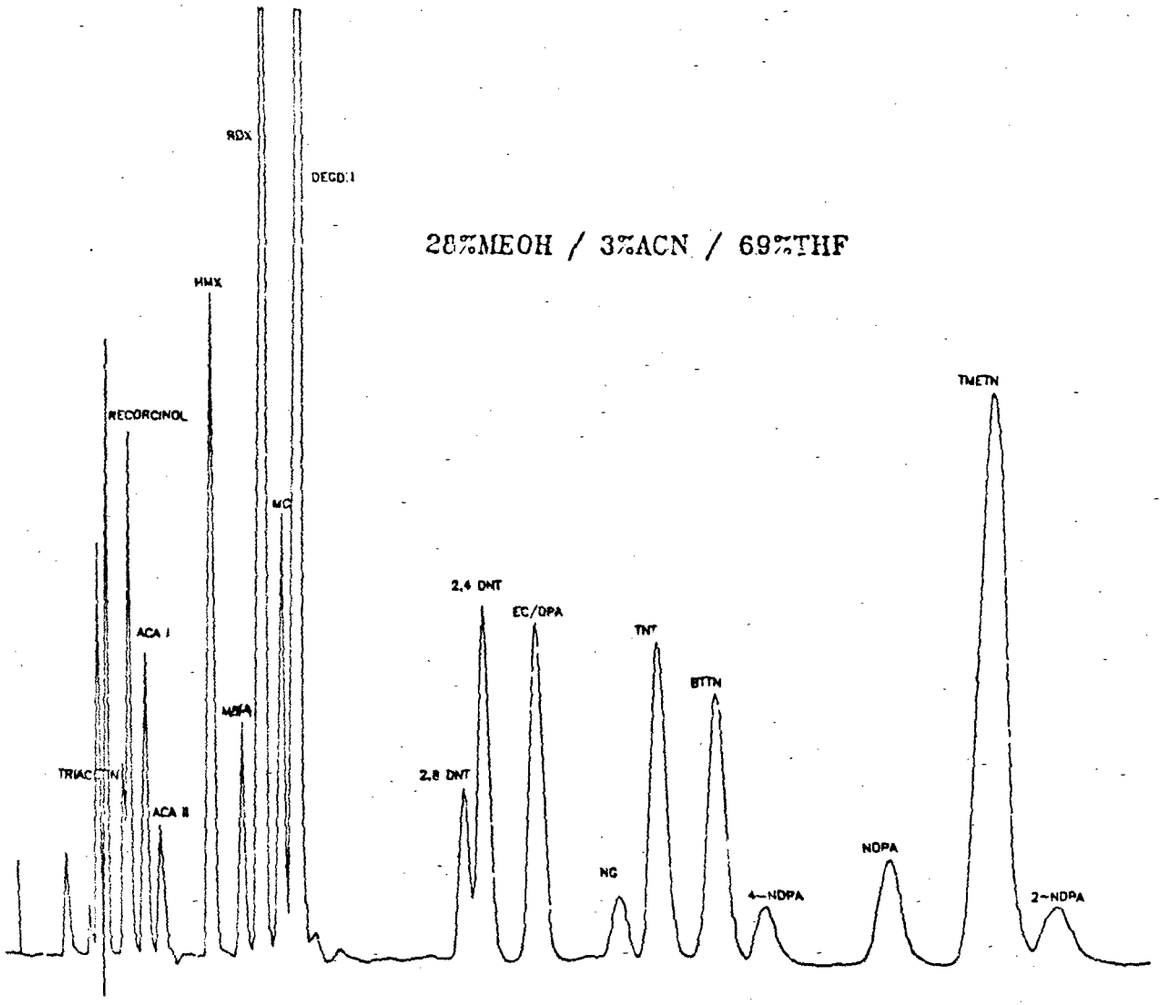

Figure 4. Waters 5 micrometer radial PAC column.

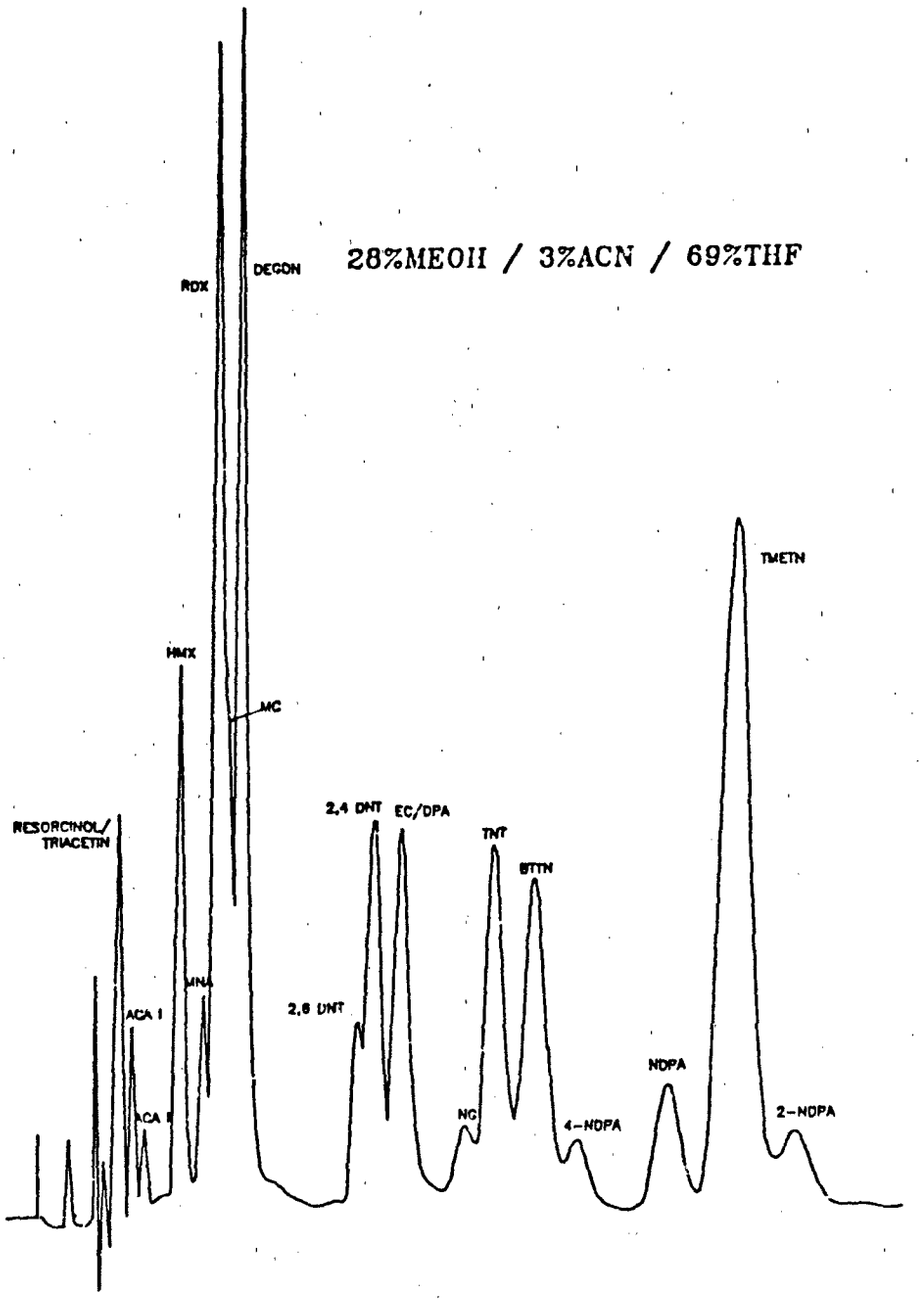

Figure 5. Waters 10 micrometer radial PAC column.

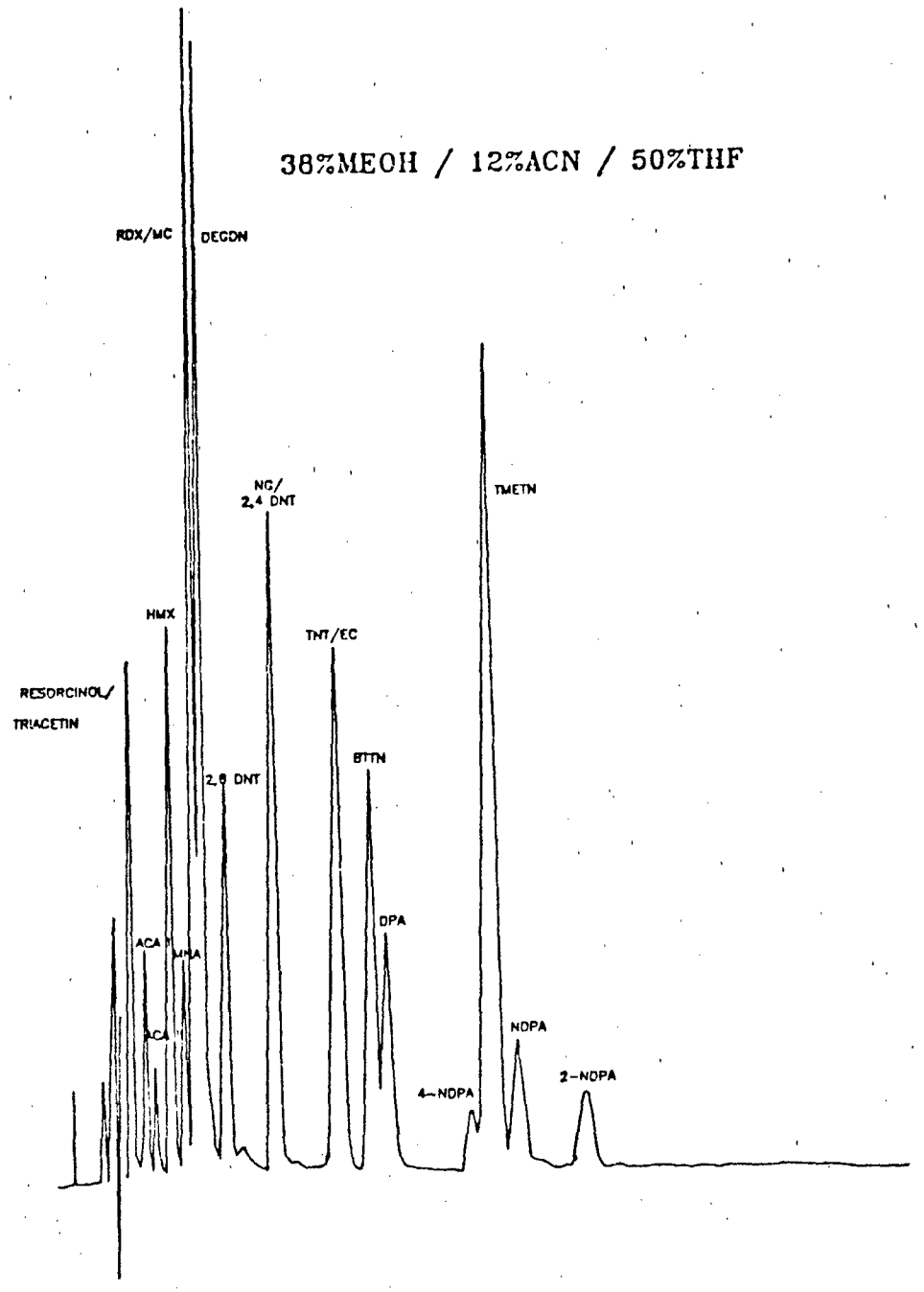

Figure 6. Perkin Elmer HS-5C-18 column.

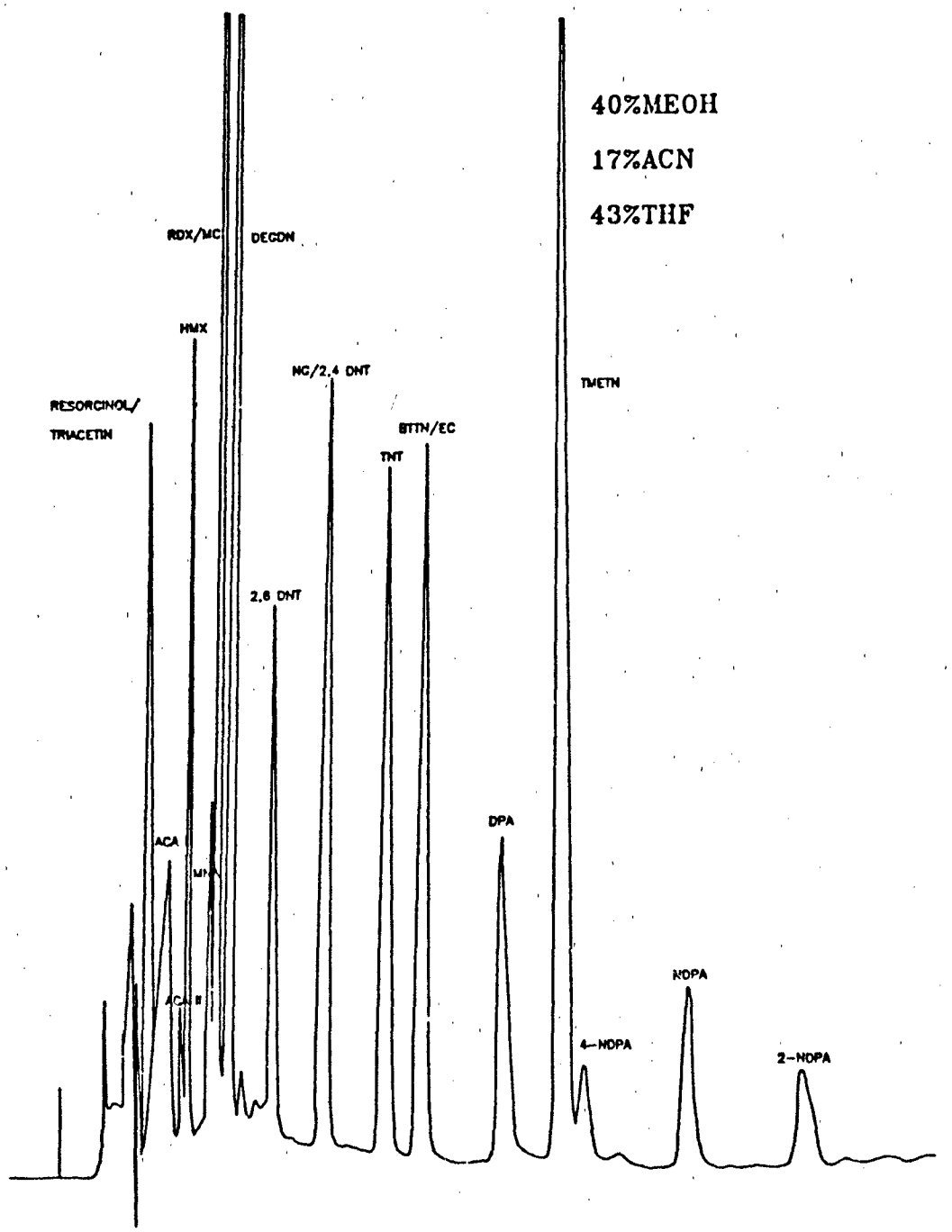

Figure 7. Suplecosil LC-18 column.

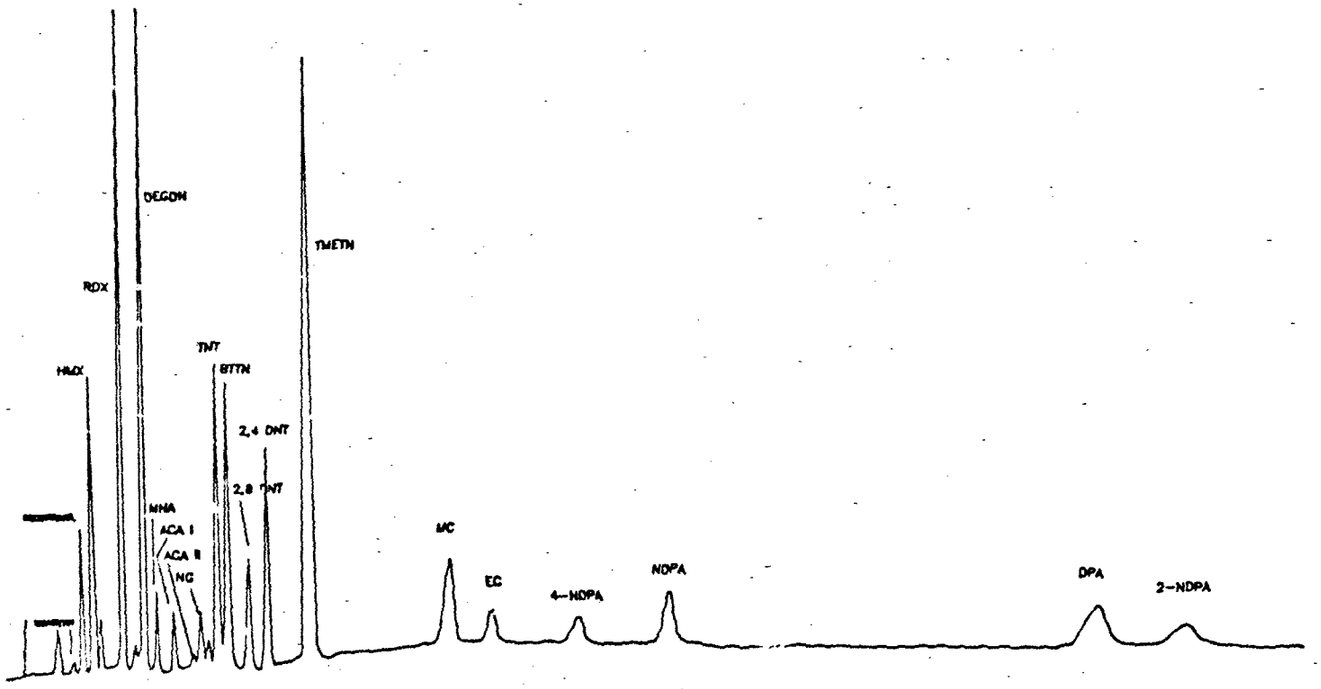

Figure 8. Dupont ODS column.

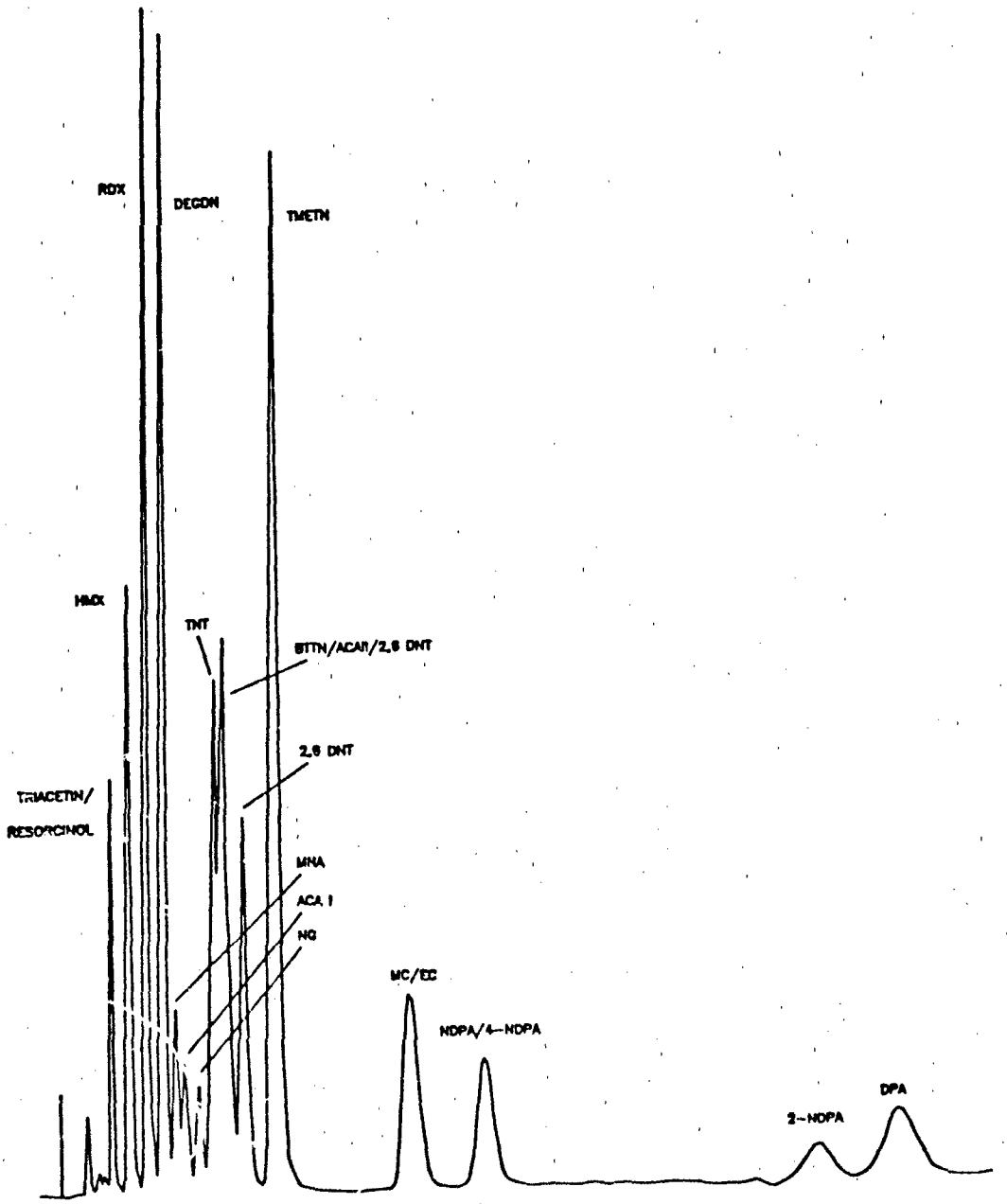

Figure 9. Waters 10 micrometer radial Pac column.

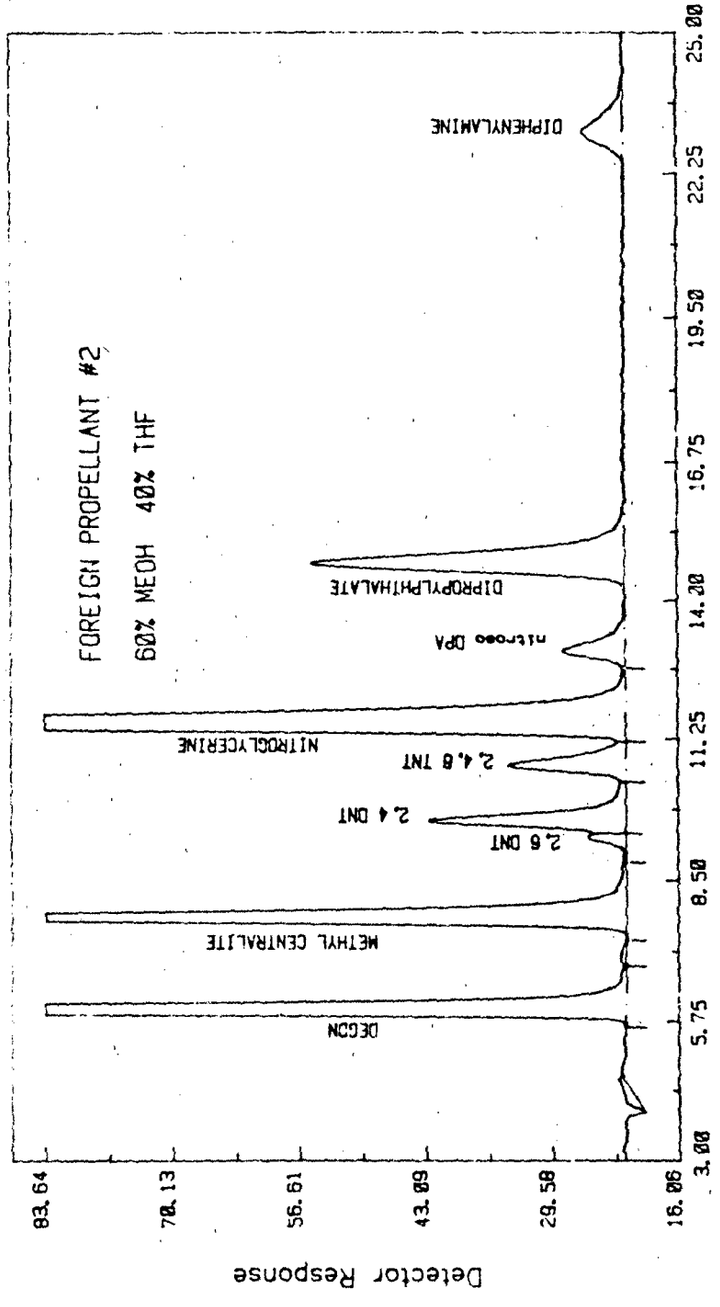

Figure 10. Foreign propellant #2.

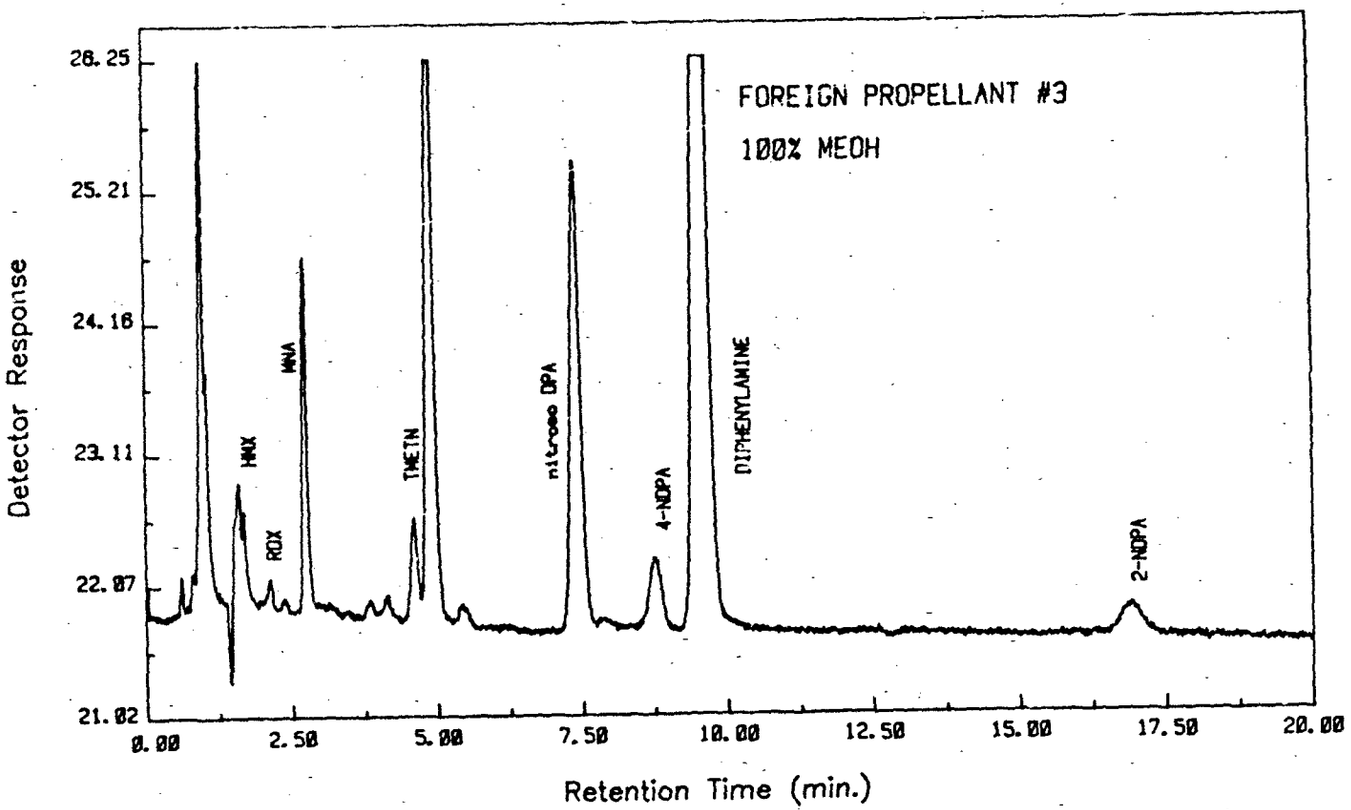

Figure 11. Foreign propellant #3.

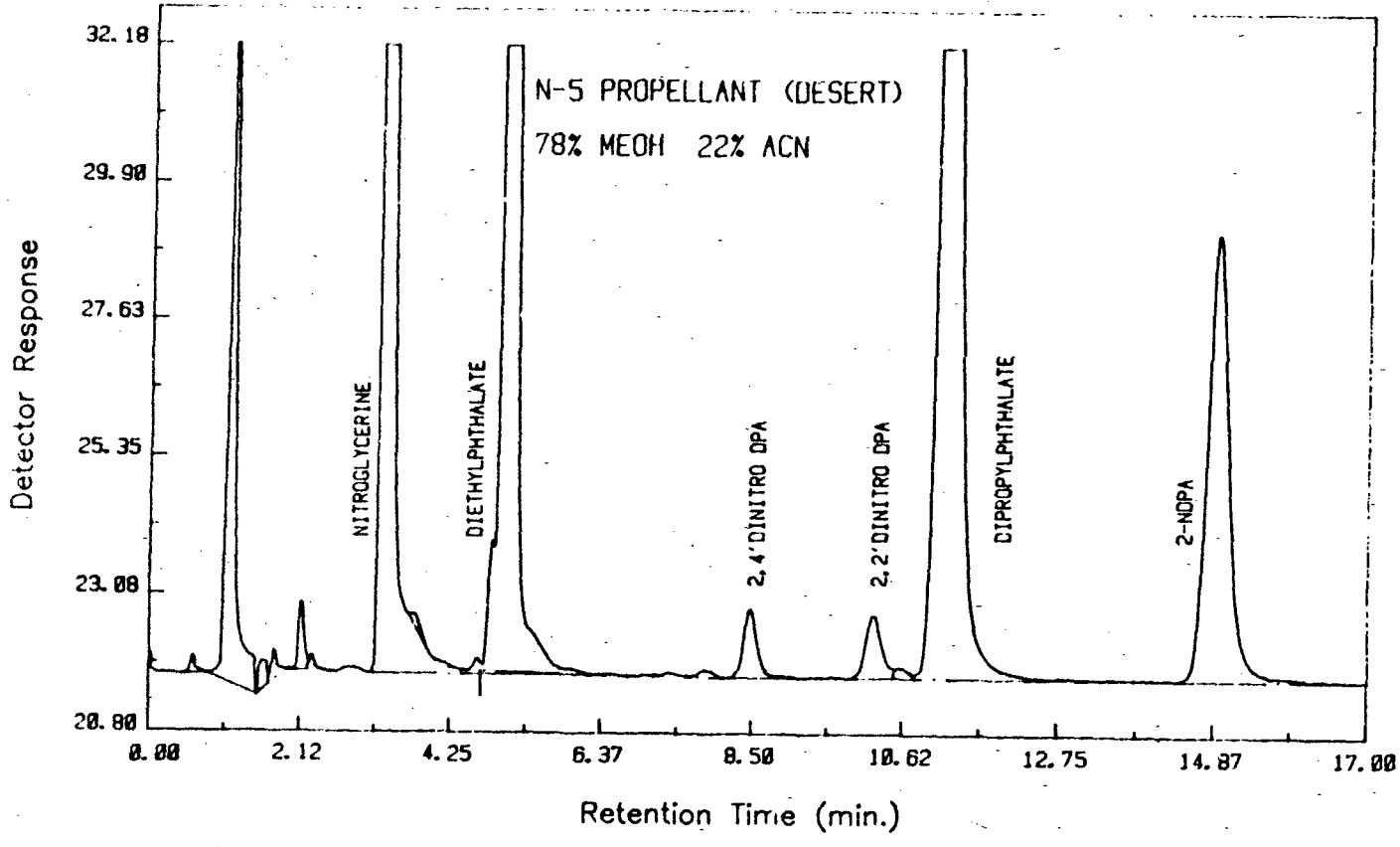

Figure 12. N-5 propellant (desert).

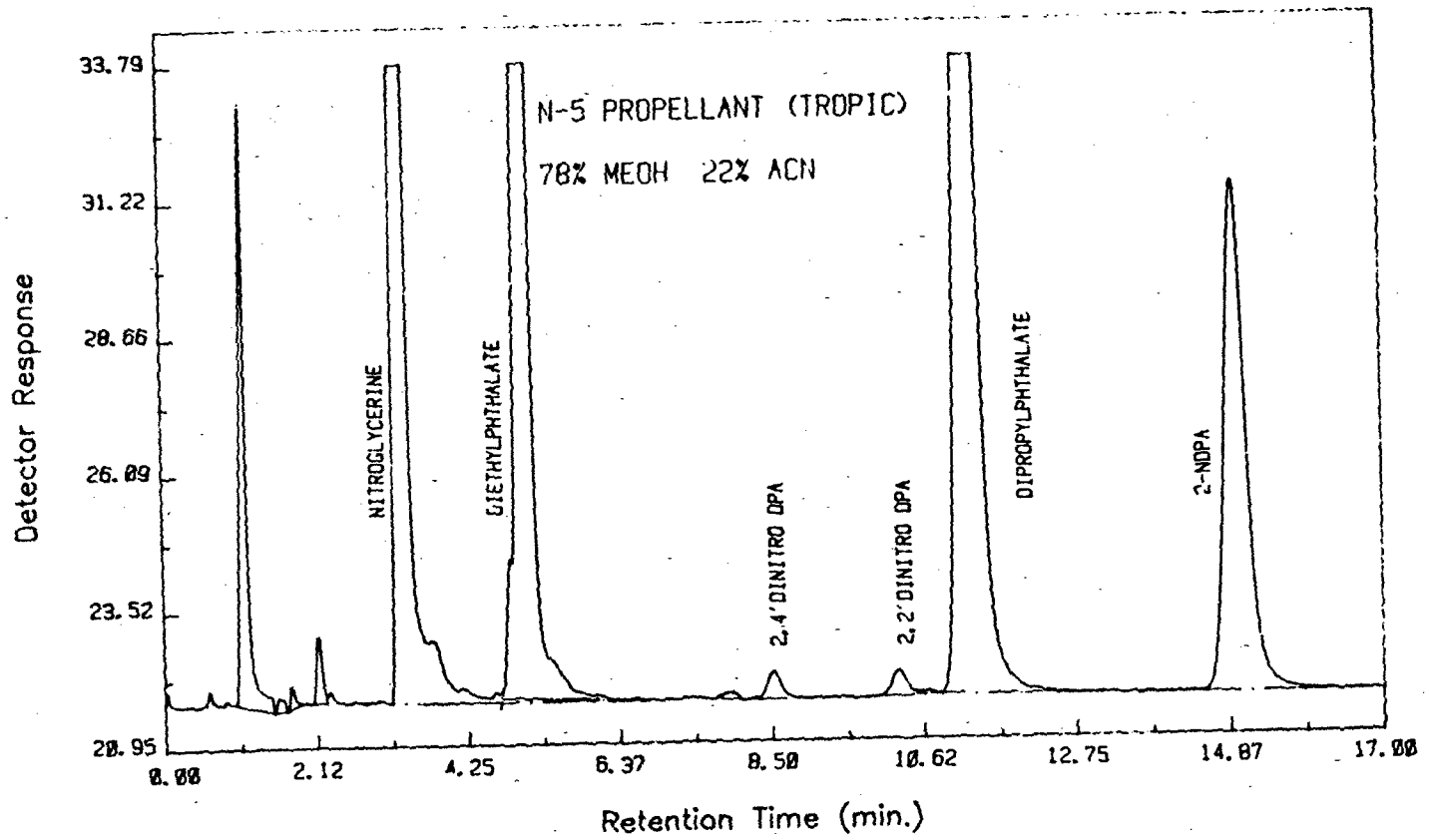

Figure 13. N-5 propellant (tropic).

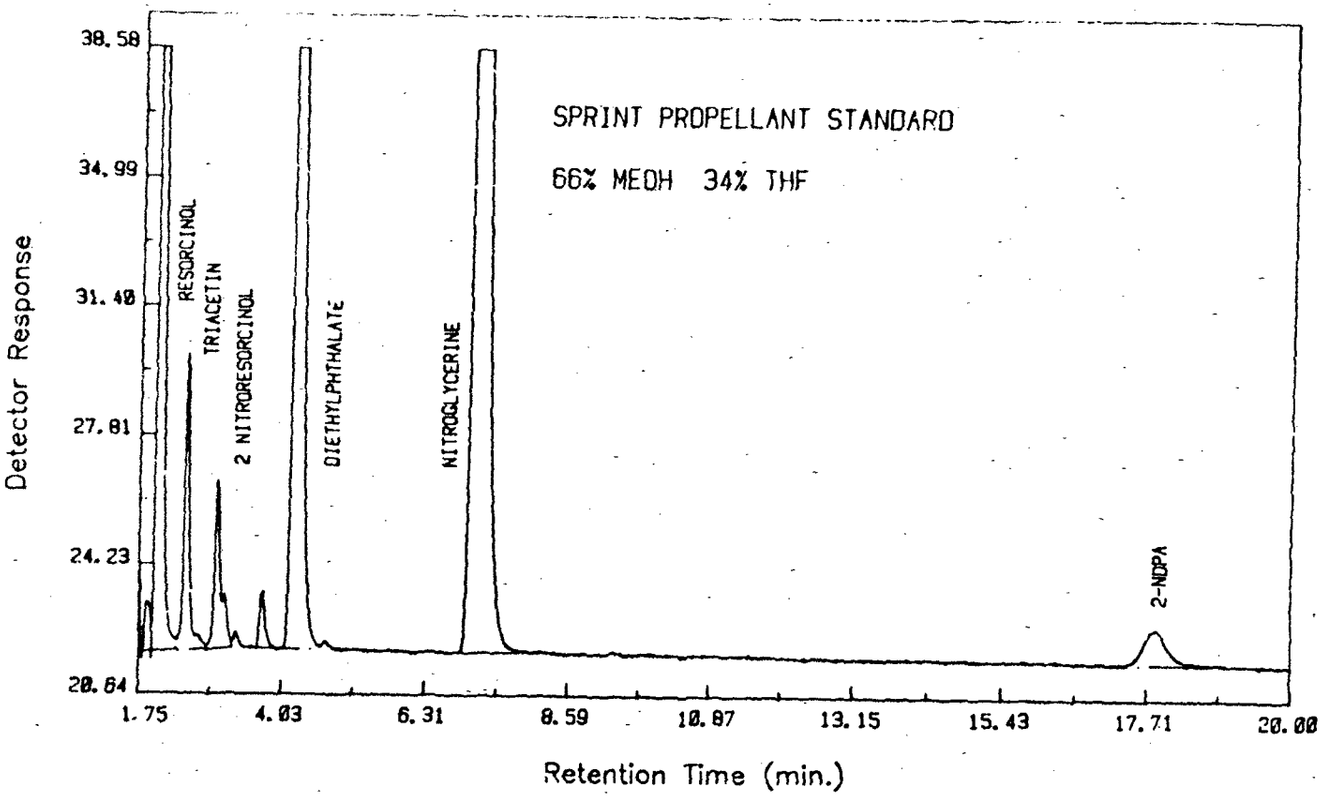

Figure 14. SPRINT propellant standard.

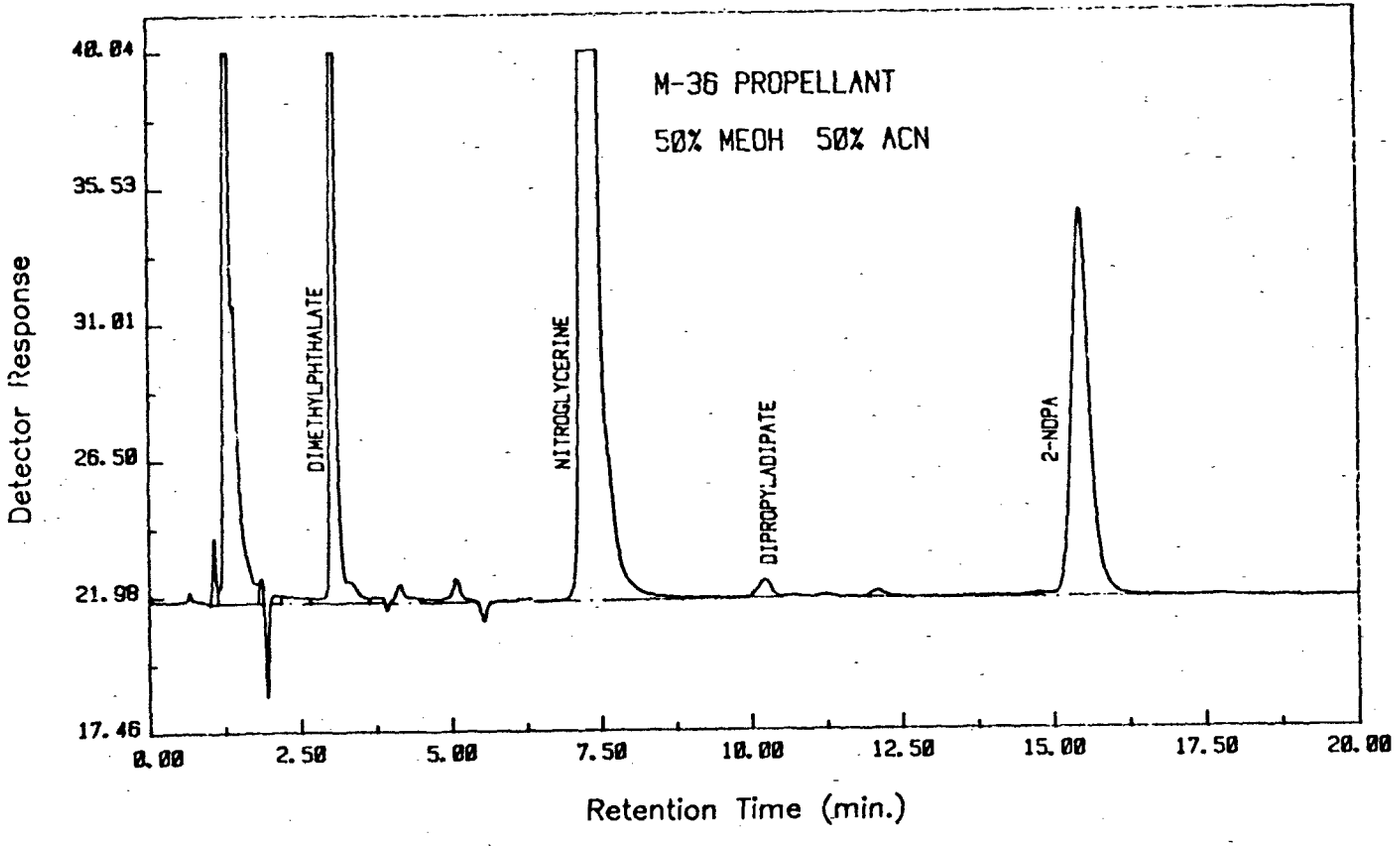

Figure 15. M-36 propellant.

LIST OF ABBREVIATIONS

HPLC	High Pressure Liquid Chromatography
GC	Gas Chromatography
MeOH	60% Methanol Water Mixture
ACN	50% Acetonitrile Water Mixture
THF	42% Tetrahydrofuran Water Mixture
DPA	Diphenylamine
NDPA	Nitrosodiphenylamine
2-NDPA	2-Nitrodiphenylamine
4-NDPA	4-Nitrodiphenylamine
2,2-DNDPA	2,2-Dinitrodiphenylamine
2,4'-DNDPA	2,4'-Dinitrodiphenylamine
2,4,4'-TNDPA	2,4,4'-Trinitrodiphenylamine
2,4-DNT	2,4-Dinitrotoluene
2,6-DNT	2,6-Dinitrotoluene
2,4,6-TNT	2,4,6-Trinitrotoluene
BTTN	1,2,4-Butanetrioltrinitrate
DEGDN	Diethyleneglycoldinitrate
DNDPA	Di-n-propyladipate
MNA	N-Methylanaline
NMNA	N-Nitroso-n-methylanaline
NG	Nitroglycerine
TIMETN	2-hydroxymethyl-2-methyl-1,3-propanedioltrinitrate

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APPENDIX A

DATA ACQUISITION

The analog out put from the detector was digitized and sent to a Hewlett-Packard Laboratory Automation System. The data was then integrated in the normal manner. A post run basic language program "PEAKWT" listed below was then automatically run. This program examines the data file for the last chromatograph. For each peak integrated, the program finds the maximum amplitude. It then samples the data points before and after the peak until it has a corrected value of 10% of the maximum. The retention time of these points are then subtracted and reported as the width of that peak.

The 10% was arbitarily selected because it is more reproducible and does not confuse a tailing peak with a very broad peak. This system gives more meaningful results when all ingredients are well separated and of approximately the same amount.

In Line 190 A$ will be returned string with the name of the raw data file and B$ the name of the processed data file. In line 240 and 250 W is the width of a data slice and N is the number of peaks integrated. In line 290 T(I) and P(I) are the retention time and amount of peak I. Line 320 sets the pointer to the first record containing extended data. Line 350 reads the height, start, baseline at start, end, and baseline at end of each peak I. The Loop in 480 to 540 finds the 10% levels at the front and end of each peak I.

```
100  REM ************************************************************
110  REM ***  BASIC PROGRAM "PEAKWT"                                ***
120  REM ***  CALCULATES PEAK WIDTH AT 10% OF THE PEAK HEIGHT.      ***
130  REM ***  TO CALCULATE AT A DIFFERENT FRACTION OF THE PEAK      ***
140  REM ***  HEIGHT CHANGE LINES 360 AND 370.                      ***
150  REM ***  CREATED BY J. CARVER 7 JUNE 1984                      ***
160  REM ************************************************************
165  COM B$[10],C$[10],M$[10],R$[10],P$[10],N[10],D[2,4],Z[4]
170  DIM N$[26],A[35],B[35],C[35],E[35],H[35],P[35],S[35],T[35],U[35]
180  FILES *,*
190  TELL A$,B$,C$,E
200  ASSIGN B$,1,E,F
210  ASSIGN C$,2,E
220  ON END #1 THEN 1000
230  ON END #2 THEN 1000
240  READ #2,1;N$,X,X,N$,X,N$,X,X,X,X,N$,N$,N$,N$,N$,X,X,W
250  READ #1,1;N$,X,X,N$,X,N$,X,X,X,X,N$,N$,N$,N$,N$,X,X,X,X,X,N
260  LET N=ABS(N)
270  READ #1,2
280    FOR I=1 TO N
290    READ #1;T[I],X,X,X,X,P[I],N$
300    NEXT I
310  LET R4=1
320  READ #1,(F/2)+2
330  READ #2,2
340    FOR I=1 TO N
350    READ #1;H[I],S[I],X,B[I],E[I],X,U[I],N$
360    LET A[I]=(H[I]*.1)+B[I]
370    LET C[I]=(H[I]*.1)+U[I]
380    LET S[I]=S[I]*60
390    LET E[I]=E[I]*60
400    LET T[I]=T[I]*60
410    LET R1=INT(S[I]/W)
420    LET R2=INT(E[I]/W)
430    LET R3=INT(T[I]/W)
440      FOR K=R4 TO R1-1
450      READ #2;N2
460      NEXT K
470    IF R4 >= R1 THEN  LET R1=R4
480      FOR K=R1 TO R2
490      READ #2;N2
500      IF K>R3 GOTO 530
510      IF N2 >= A[I] AND INT(S[I]/W)=R1 THEN  LET S[I]=K*W
520      GOTO 540
530      IF N2 <= C[I] AND INT(E[I]/W)=R2 THEN  LET E[I]=K*W
540      NEXT K
550    LET R4=R2+1
560    NEXT I
1000 PRINT
1010 PRINT
1020 PRINT "PROCESSED FILE ";B$
1030 PRINT
1040 PRINT TAB(30);"10% OF HEIGHT"
1050 PRINT "PEAK RT","AREA % ","PEAK WIDTH (SEC)"
1060 PRINT
1070   FOR I=1 TO N
1080   LET W=(E[I]-S[I])
1090   LET T[I]=T[I]/60
1100   PRINT T[I],P[I],W
1110   NEXT I
1120 PRINT
1130 PRINT
1140 PRINT
1150 END
```

APPENDIX B

DATA REDUCTION BASIC LANGUAGE VERSION

The basic language version of the data reduction was designed to output to a Hewlett-Packard 2648 graphics terminal with a 9876 A graphics printer attached as a "C" device.

Line 145 to 155 in program XLDB6A open previously created data files to the program. These 7 files contain the retention data from the 7 solvent compositions. This program can enter new data or change old data in these files. It can not create the files. This must be done separately by the user. When the files are satisfactory, the user can list the data input as well as the resolution for pairs of peaks in each solvent. A chromatographic optimization function, as discussed by Synder [21], is also calculated. The program then calls XLDB6B for further calculations and plotting lines of resolution for each peak pair on the graphics terminal.

```
10  COM M[2],T[7,35]
100  REM ****************************************************
105  REM *********LIQUID CHROMATOGRAPHIC OPTIMIZATION******
110  REM *********** XLDB6A **R.RADKE / J.CARVER ***********
115  REM ************************AUG/SEPT 1981*************
120  REM ****************************************************
125  LET M1=7
130  LET M2=8
135  DIM E$[1],S[7],V[7],W[7,35],K[7,35],R[7,35]
140  CHR$ 27,E$
145  FILES FIRST::19,SECOND::19,THIRD::19
150  FILES FOURTH::19,FIFTH::19,SIXTH::19
155  FILES SEVNTH::19
160  REM GET SOLVENTS
165  PRINT
170  PRINT " ENTER THE NUMBER OF SOLVENTS (1-7)  <0=EXIT>"
175  INPUT M1
180  IF M1=0 THEN 9999
185  IF M1<1 THEN 170
190  IF M1>7 THEN 170
195  LET M[1]=M1
200  REM GET PEAKS
205  PRINT " ENTER THE NUMBER OF PEAKS PER SOLVENT (2-35)  <0=EXIT>"
210  INPUT M2
215  IF M2=0 THEN 9999
220  IF M2<2 THEN 205
225  IF M2>35 THEN 205
230  LET M[2]=M2
235  REM LOOP TO GET DATA
240    FOR J=1 TO M1
245    PRINT " ENTER THE RETENTION TIME (MIN) FOR SOLVENT ";J;" <0=EXIT>"
250    INPUT V[J]
255    IF V[J]=0 THEN 9999
260    LET V[J]=V[J]*60
265    PRINT " ENTER THE AVERAGE BAND WIDTH <SEC> FOR ALL PEAKS OF SOLVENT ";J
270    INPUT A
275      FOR I=1 TO M2
280      PRINT " ENTER THE RETENTION TIME (MIN) FOR PEAK ";I;" <0=EXIT>"
285      INPUT T[J,I]
290      IF T[J,I]=0 THEN 9999
295      LET T[J,I]=T[J,I]*60
300      LET W[J,I]=A
305      LET K[J,I]=(T[J,I]-V[J])/V[J]
310      NEXT I
315    NEXT J
320  GOSUB 605
325  REM CALCULATE THE RESOLUTION
330  GOSUB 6000
335    FOR J=1 TO M1
340      FOR I=1 TO M2-1
345        FOR K=I+1 TO M2
350        LET A=(T[J,K]-T[J,I])/(.5*(W[J,K]+W[J,I]))
355        PRINT #J;A
360        NEXT K
365      NEXT I
370    NEXT J
375  REM *** CALCULATE RESPONSE FUNCTION ***
380  PRINT " ENTER DESIRED RESOLUTION  <0=GO TO ORM>"
385  INPUT R9
390  IF R9=0 THEN  CHAIN "XLDB6B"
```

```
395  IF R9<0 THEN 380
400  GOSUB 6000
405    FOR J=1 TO M1
410    LET S[J]=0
415      FOR I=1 TO M2-1
420        FOR K=I+1 TO M2
425        READ #J;A
430        LET Z=A/R9
435        IF Z <= 0 THEN 445
440        LET S[J]=S[J]+LN(Z)
445        NEXT K
450      NEXT I
455    NEXT J
460  REM *** OUTPUT TABLE ***
465  GOSUB 6000
470    FOR J=1 TO M1
475    OUTDVC "C1",E
480    PRINT E$"U"
485    PRINT " RETENTION TIME FOR SOLVENT ";J;" IS ";(V[J]/60);" MIN"
490    PRINT
495    PRINT
500    PRINT " PEAK"," RETEN TIME"," BAND WIDTH"," CAPACITY"
505      FOR I=1 TO M2
510      PRINT TAB(3);I;TAB(19);(T[J,I]/60);TAB(34);W[J,I];TAB(47);K[J,I]
515      NEXT I
520    PRINT
525    PRINT
530    PRINT " FOR PEAKS"," RESOLUTION"
535    PRINT
540      FOR I=1 TO M2-1
545        FOR K=I+1 TO M2
550        READ #J;A
555        PRINT TAB(3);I;"- ";K;TAB(17);A
560        NEXT K
565      NEXT I
570    PRINT
575    PRINT
580    PRINT " CHROMATOGRAPHIC OPTOMIZATION FUNCTION (COF) FOR SOLVENT ";J;
585    PRINT " IS ";S[J]
590    NEXT J
595  OUTDVC "T*",E
600  CHAIN "XLOB69"
605  REM PRINT INPUT
610  PRINT
615  PRINT
620  PRINT TAB(8)"SOLVENT-1 SOLVENT-2 SOLVENT-3 SOLVENT-4 SOLVENT-5";
625  PRINT TAB(58)"SOLVENT-6 SOLVENT-7"
630  PRINT TAB(8)"-------------------------------------------------";
635  PRINT TAB(58)"--------------------"
640  PRINT "T0";
645    FOR X=1 TO M1
650    PRINT TAB(X*10-2);V[X]/60;
655    NEXT X
660  PRINT
665  PRINT "WIDTH";
670    FOR X=1 TO M1
675    PRINT TAB(X*10-2);W[X,1];
680    NEXT X
685  PRINT
690    FOR Y=1 TO M2
```

```
695  PRINT "RT-"Y;
700    FOR X=1 TO M1
705    PRINT TAB(X*10-2);T[X,Y]/60;
710    NEXT X
715  PRINT
720  NEXT Y
725  PRINT TAB(8);"-------------------------------------------------------";
730  PRINT TAB(58);"-----------------"
735  PRINT
740  PRINT "ARE THERE ANY CHANGES";
745  INPUT C$
750  IF C$[1,1]="Y" THEN 1000
755  RETURN
1000 REM MAKE CHANGES
1005 PRINT "WHICH SOLVENT (1-";M1;")";
1010 INPUT J
1015 PRINT "TO=";V[J]/60;"  THE NEW VALUE IS";
1020 INPUT V[J]
1025 LET V[J]=V[J]*60
1030 PRINT "WIDTH =";W[J,1];"  THE NEW VALUE IS";
1035 INPUT A
1040   FOR X=1 TO M2
1045   LET W[J,X]=A
1050   NEXT X
1055 PRINT "WHICH PEAK NEEDS TO BE CHANGED (1-";M2;")";
1060 INPUT I
1065 PRINT "PEAK ";I;"HAS A RETENTION TIME OF ";T[J,I]/60;" THE NEW VALUE IS";
1070 INPUT T[J,I]
1075 LET T[J,I]=T[J,I]*60
1080 LET K[J,I]=(T[J,I]/V[J])-1
1085 PRINT
1090 PRINT "ANY MORE CHANGES FOR SOLVENT ";J;
1095 INPUT C$
1100 IF C$[1,1]="Y" THEN 1055
1105 PRINT "ANY CHANGES FOR ANOTHER SOLVENT";
1110 INPUT C$
1115 IF C$[1,1]="Y" THEN 1005
1120 GOSUB 610
1125 GOTO 325
6000 REM *** RESET POINTERS ***
6005 READ #1,1
6010 READ #2,1
6015 READ #3,1
6020 READ #4,1
6025 READ #5,1
6030 READ #6,1
6035 READ #7,1
6040 RETURN
9999 END
```

```
10  COM A[2],T[7,35]
100  REM ******************************************************
105  REM *********LIQUID CHROMATOGRAPHIC OPTIMIZATION******
110  REM *********** XLDB6B **R.RADKE / J.CARVER **********
115  REM ***************************AUG/SEPT 1981***********
120  REM ******************************************************
125  CHRS 27,E$
130  DIM E$[1],Y$[10],Z$[26],B[35],C[35]
135  LET Y$="0123456789"
140  LET Z$="      ,              :   AM"
145  LET M[1]=M[3]=M[5]=M[7]=M[8]=M[10]=M[12]=31
150  LET M[4]=M[6]=M[9]=M[11]=30
155  LET M[2]=28
160  FILES FIRST::19,SECOND::19,THIRD::19
165  FILES FOURTH::19,FIFTH::19,SIXTH::19
170  FILES SEVNTH::19,RESOLV::19,HOLDER::19
175  READ #8,1
180    FOR I1=0 TO 100 STEP 2
185      FOR J1=0 TO 100-I1 STEP 2
190      PRINT #8;1.00000E+38
195      NEXT J1
200    NEXT I1
2000  REM *** ORM SUBROUTINE ***
2005  OUTDVC "T*",E
2010  LET M1=A[1]
2015  LET M2=A[2]
2020  GOSUB 6000
2025    FOR I=1 TO M2-1
2030    PRINT "WORKING!"
2035      FOR K=I+1 TO M2
2040      GOSUB 6100
2045      LET V=0
2050      GOSUB 3000
2055      NEXT K
2060    NEXT I
2065  OUTDVC "L2",E
2070  PRINT E$"U"
2075  PRINT
2080  PRINT
2085  GOSUB 5000
2090  PRINT TAB(20)"HPLC DATA ANALYSIS"
2095  PRINT TAB(20)"RUN ";S[2];D$[S[3]-3,S[3]];S[4]
2100  GOSUB 3300
2105  GOSUB 3500
2110  OUTDVC "T*",E
2115  PRINT
2120  PRINT "DO YOU WANT TO PLOT LINES OF RESOLUTION? (Y/N)";
2125  INPUT C$
2130  IF C$[1,1]#"Y" THEN  STOP
2135  PRINT
2140  PRINT "WHAT IS THE MINIMUM RESOLUTION DESIRED ";
2145  INPUT R9
2150  PRINT "PEAK PAIRS ALWAYS RESOLVED GREATER THAN ";R9;"WILL BE IGNORED."
2155  OUTDVC "C1",E
2160  PRINT E$"U"
2165  LET Z1=2
2170  REM *** GET Y AND BETA VALUES ***
2175  GOSUB 6000
2180    FOR I=1 TO M2-1
2185      FOR K=I+1 TO M2
```

```
2190  GOSUB 6100
2195  PRINT
2200  PRINT
2205  PRINT
2210  REM *** CHECK FOR R9,-R9, AND 0 ***
2215  OUTDVC "T*",E
2220  PRINT E$"H",E$"J"
2225  PRINT " FOR PEAK PAIR ";I;"- ";K
2230  LET R7=Y=0
2235  PRINT "CHECKING FOR RESOLUTION OF ";Y
2240  GOSUB 5500
2245  IF R7=1 THEN 2295
2250  LET Y=R9
2255  PRINT "CHECKING FOR RESOLUTION OF ";Y
2260  GOSUB 5500
2265  IF R7=1 THEN 2295
2270  LET Y=-R9
2275  PRINT "CHECKING FOR RESOLUTION OF ";Y
2280  GOSUB 5500
2285  IF R7=1 THEN 2295
2290  IF Z1=3 THEN  GOSUB 5700
2295  REM *** PRINT HEADING ***
2300  PRINT E$"b"
2305  OUTDVC "C1",E
2310  IF R7=1 THEN  PRINT E$"U"
2315  PRINT
2320  PRINT
2325  PRINT " FOR PEAK PAIR ";I;"- ";K
2330  PRINT
2335  PRINT " BETA COEFFICIENTS (1-7)"
2340  PRINT B1;B2;B3;B4;B5;B6;B7
2345  PRINT
2350  PRINT
2355  REM *** CHECK POINTS ***
2360  PRINT "  MEOH","ACN","THF","Y"
2365  PRINT "-------------------------------------------------------"
2370  LET X1=X2=.16
2375  LET X3=.68
2380  GOSUB 5800
2385  LET X1=X3=.16
2390  LET X2=.68
2395  GOSUB 5800
2400  LET X1=.68
2405  LET X2=X3=.16
2410  GOSUB 5800
2415  LET X1=X2=0
2420  LET X3=1
2425  GOSUB 5800
2430  LET X1=X3=0
2435  LET X2=1
2440  GOSUB 5800
2445  LET X1=1
2450  LET X2=X3=0
2455  GOSUB 5800
2460  PRINT "-------------------------------------------------------"
2465  PRINT
2470  PRINT
2475  IF R7=1 THEN  LET Z1=0
2480  LET Z1=Z1+1
2485  IF R7=1 THEN  GOSUB 4000
```

```
2490  IF R7=1 THEN  PRINT E$"&p5D"E$"&p5u0C"
2495  IF R7#1 THEN  PRINT "PEAK PAIR ";I;"- ";K;"IS ALWAYS RESOLVED ";R9
2500  IF R7=1 THEN  GOSUB 5700
2505  NEXT K
2510  NEXT I
2515  OUTDVC "T*",E
2520  PRINT E$"b"
2525  PRINT "DO YOU WANT TO PLOT A DIFFERENT RESOLUTION (Y/N)";
2530  INPUT C$
2535  IF C$[1,1]="Y" THEN 2140
2540  STOP
3000  REM *** CALCULATES BEST SEPARATION SOLVENT ***
3005  READ #8,1
3010  READ #9,1
3015    FOR I1=0 TO 100 STEP 2
3020      FOR J1=0 TO 100-I1 STEP 2
3025      LET X1=I1/100
3030      LET X2=J1/100
3035      LET X3=1-X1-X2
3040      LET Y=B1*X1+B2*X2+B3*X3+B4*X1*X2+B5*X1*X3+B6*X2*X3+B7*X1*X2*X3
3045      READ #8;Y1
3050      IF ABS(Y) <= Y1 THEN  LET Y1=ABS(Y)
3055      PRINT #9;Y1
3060      IF Y1 <= V THEN 3080
3065      LET V=Y1
3070      LET X6=I1
3075      LET X7=J1
3080      NEXT J1
3085    NEXT I1
3090  READ #8,1
3095  READ #9,1
3100    FOR I1=0 TO 100 STEP 2
3105      FOR J1=0 TO 100-I1 STEP 2
3110      READ #9;Y
3115      PRINT #8;Y
3120      NEXT J1
3125    NEXT I1
3130  RETURN
3300  REM *** PRINT BEST SEPARATION ***
3305  LET X1=X6/100
3310  LET X2=X7/100
3315  LET X3=1-X1-X2
3320  PRINT
3325  PRINT
3330  PRINT
3335  PRINT TAB(15);"THE BEST COMPOSITION IS:"
3340  PRINT
3345  PRINT TAB(10);"MEOH";TAB(25);"ACN";TAB(40);"THF"
3350  PRINT TAB(11);X6;"%";TAB(25);X7;"%";TAB(41);(100-X6-X7);"%"
3355  PRINT
3360  PRINT TAB(5);"THE WORST RESOLUTION AT THIS POINT IS ";V
3365  PRINT
3370  PRINT
3375  RETURN
3500  REM *** PREDICT ORDER OF ELUTION ***
3505  GOSUB 6000
3510  LET I=C[1]=1
3515  LET W=20
3520  LET B[1]=T[1,1]
3525    FOR K=2 TO M2
```

```
3530  LET C[K]=K
3535  GOSUB 6100
3540  LET Y=B1*X1+B2*X2+B3*X3+B4*X1*X2+B5*X1*X3+B6*X2*X3+B7*X1*X2*X3
3545  LET B[K]=W*Y+B[1]
3550  NEXT K
3555  REM *** SORT ***
3560    FOR I=1 TO M2-1
3565      FOR J=I+1 TO M2
3570      IF B[J] >= B[I] THEN 3605
3575      LET B1=B[I]
3580      LET C1=C[I]
3585      LET C[I]=C[J]
3590      LET C[J]=C1
3595      LET B[I]=B[J]
3600      LET B[J]=B1
3605      NEXT J
3610    NEXT I
3615  PRINT TAB(15);"PREDICTED ORDER OF ELUTION"
3620  PRINT
3625  PRINT TAB(10);"PEAK # ","RELATIVE RETENTION TIME"
3630  PRINT
3635    FOR I=1 TO M2
3640    PRINT TAB(10);C[I];TAB(35);B[I]/60
3645    NEXT I
3650  RETURN
4000  REM PLOT GRID
4001  OUTDVC "C1",E
4002  PRINT
4003  PRINT
4004  PRINT
4005  PRINT
4007  OUTDVC "T*",E
4010  DIM I[21],J[21],L[21],M[21],N[21],O[21]
4030  LET G1=10
4040  LET G2=400
4050  LET K1=11
4060  LET D=G2/(K1-1)
4070    FOR I1=1 TO K1
4080    LET A=I1-1
4090    LET I[I1]=INT(G1+(0*G2+(1)*A*D)/1)
4100    LET J[I1]=INT(G1+(2*G2+(-1)*A*D)/2)
4110    LET L[I1]=INT(G1+(1*G2+(-1)*A*D)/2)
4120    LET M[I1]=INT(G1+(0*G2+(0)*A*D)*SQR(3)/2)
4130    LET N[I1]=INT(G1+(0*G2+(1)*A*D)*SQR(3)/2)
4140    LET O[I1]=INT(G1+(1*G2+(-1)*A*D)*SQR(3)/2)
4150    NEXT I1
4160  REM PRINT GRID
4170  PRINT E$"H"E$"J"E$"*m2a 0,0 jibZ"E$"*dachlntZ"
4180  LET M=K1-1
4190    FOR N=1 TO M
4200    LET L=N+1
4210    LET J=K1-N
4220    PRINT E$"*pah"I[L],M[L]"Z"E$"*pbh"L[J],O[J]"Z"
4230    PRINT E$"*pah"J[L],N[L]"Z"E$"*pbh"I[J],M[J]"Z"
4240    PRINT E$"*pah"L[L],O[L]"Z"E$"*pbh"J[J],N[J]"Z"
4250    NEXT N
4260  PRINT E$"*d0,0okSTHF"
4270  PRINT E$"*d422,0OACN"
4280  PRINT E$"*d230,350OMEOH"
4290  PRINT E$"*dlT"
```

```
4300  REM  *** PLOT LINES OF RESOLUTION ***
4302  DIM X[101],Y[101],P[101],Q[101]
4303  LET Y=R9
4304  GOSUB 4310
4305  LET Y=-R9
4306  GOSUB 4310
4307  LET Y=0
4308  GOSUB 4310
4309  RETURN
4310  LET N=M=1
4311    FOR X=0 TO 100
4312    LET X1=X/100
4314    LET C1=B3+(B1-B3+B5-B5*X1)*X1
4316    LET C2=B2-B3+B6+(B4-B5-B6+B7-B7*X1)*X1
4318    LET C3=0-B6-B7*X1
4320    LET A=C3
4322    LET B=C2
4324    LET C=C1-Y
4326    LET D=B*B-4*A*C
4328    IF D<0 THEN 4370
4330    LET S=SQR(D)
4332    LET R1=(0-B+S)/(2*A)
4334    LET R2=(0-B-S)/(2*A)
4336    IF R1<0 THEN 4352
4338    IF R1>1 THEN 4352
4340    LET Q1=X1+R1
4342    IF Q1>1 THEN 4352
4344    LET X2=1-Q1
4346    LET X3=R1
4348    LET X[N]=G1+(X3+X1/2)*G2
4350    LET Y[N]=G1+X1*G2*SQR(3)/2
4351    LET N=N+1
4352    IF R2<0 THEN 4370
4354    IF R2>1 THEN 4370
4356    LET Q2=X1+R2
4358    IF Q2>1 THEN 4370
4360    LET X2=1-Q2
4362    LET X3=R2
4364    LET P[M]=G1+(X3+X1/2)*G2
4366    LET Q[M]=G1+X1*G2*SQR(3)/2
4368    LET M=M+1
4370    NEXT X
4372  IF N<3 THEN 4392
4374  LET Y8=Y[1]
4376  LET X8=X[1]
4378    FOR I9=2 TO N-1
4380    LET X9=X[I9]
4382    LET Y9=Y[I9]
4384    PRINT E$"*pah"X8,Y8"Z"E$"*pbh"X9,Y9"Z"
4386    LET X8=X9
4388    LET Y8=Y9
4390    NEXT I9
4391  PRINT E$"*dsZ";Y
4392  PRINT E$"*dtZ"
4393  IF M<3 THEN  RETURN
4394  LET Y8=Q[1]
4396  LET X8=P[1]
4398    FOR I9=2 TO M-1
4400    LET X9=P[I9]
4402    LET Y9=Q[I9]
```

```
4404  PRINT E$"*pah"X8,Y8"Z"E$"*pbh"X9,Y9"Z"
4406  LET X8=X9
4408  LET Y8=Y9
4410  NEXT I9
4412  PRINT E$"*dsZ"
4413  PRINT Y
4414  PRINT E$"*dtZ"
4416  RETURN
5000  REM *** GET DATE AND TIME ***
5010  DIM D$[48]
5020  LET D$="JAN FEB MAR APR MAY JUNEJULYAUG SEPTOCT NOV DEC "
5021  LET Z2=TIM(3)
5022  LET Z3=9
5023  LET Z4=12
5024  IF Z2/400=INT(Z2/400) LET M[2]=29
5025  IF Z2/100#INT(Z2/100) AND Z2/4=INT(Z2/4) LET M[2]=29
5026  LET Z2=TIM(2)
5027    FOR Z=1 TO 12
5028    LET Z2=Z2-M[Z]
5029    IF Z2 <= 0 THEN 5031
5030    NEXT Z
5031  LET S[2]=Z2+M[Z]
5040  LET S[4]=TIM(3)
5060  LET S[3]=Z*4
5070  RETURN
5500  REM *** CALCULATES PREDICTED RESOLUTION VALUES ***
5502  PRINT E$"c"
5504    FOR X=0 TO 100 STEP 2
5506    LET X1=X/100
5508    LET C1=B3+(B1-B3+B5-B5*X1)*X1
5510    LET C2=B2-B3+B6+(B4-B5-B6+B7-B7*X1)*X1
5512    LET C3=0-B6-B7*X1
5514    LET A=C3
5516    LET B=C2
5518    LET C=C1-Y
5520    LET D=B*B-4*A*C
5522    IF D<0 THEN 5548
5524    LET S=SQR(D)
5526    LET R1=(0-B+S)/(2*A)
5528    LET R2=(0-B-S)/(2*A)
5530    IF R1<0 OR R1>1 THEN 5538
5532    LET Q1=X1+R1
5534    IF Q1>1 THEN 5538
5536    LET R7=1
5538    IF R2<0 OR R2>1 THEN 5546
5540    LET Q2=X1+R2
5542    IF Q2>1 THEN 5546
5544    LET R7=1
5546    IF R7=1 THEN  RETURN
5548    NEXT X
5550  RETURN
5700  REM *** NEW PAGE ***
5702  OUTDVC "C1",E
5704  PRINT E$"U"
5706  LET Z1=1
5708  RETURN
5800  REM *** CALCULATE PREDICTED RESOLUTION VALUES ***
5802  LET Y=B1*X1+B2*X2+B3*X3+B4*X1*X2+B5*X1*X3+B6*X2*X3+B7*X1*X2*X3
5804  PRINT X1*100,X2*100,X3*100,Y
5806  RETURN
```

```
6000  REM *** RESET POINTERS ***
6005  READ #1,1
6010  READ #2,1
6015  READ #3,1
6020  READ #4,1
6025  READ #5,1
6030  READ #6,1
6035  READ #7,1
6040  RETURN
6100  REM *** GET BETA COEFFICIENTS ***
6105  READ #1;Y1
6110  READ #2;Y2
6115  READ #3;Y3
6120  READ #4;Y4
6125  READ #5;Y5
6130  READ #6;Y6
6135  READ #7;Y7
6140  REM SOLVE FOR BETA COEFFICIENTS
6145  LET B1=Y1
6150  LET B2=Y2
6155  LET B3=Y3
6160  LET B4=4*Y4-2*(Y1+Y2)
6165  LET B5=4*Y5-2*(Y1+Y3)
6170  LET B6=4*Y6-2*(Y2+Y3)
6175  LET B7=27*Y7-12*(Y4+Y5+Y6)+3*(Y1+Y2+Y3)
6180  RETURN
9999  END
```

APPENDIX C

DATA REDUCTION FORTRAN 77 VERSION

This is basically a translated version of XLDB6A and B but with many enhancements. It still has a section to plot lines of resolution on a Hewlett-Packard graphics terminal with a graphics printer capable of a RASTER Dump but it is not limited to a graphics terminal. Extensive use of the Hewlett-Packard graphics package "DGL" has been made. This allows the user to use a 4 pen graphics plotter for output from a nongraphics terminal. Figure 1 of report text is typical of the output. This greatly simplifies selection of a solvent. Another enhancement is that the output gives expected retention time of named peaks for any selected composition and the minimum resolution predicted at that composition. Table 3 of report text is an example of this output.

```
$FILES 2,3
$ENA /TWO/,/THREE/,/FOUR/,/SIX/
*****************************************************************************
*                          VARIABLE IDENTIFICATION                          *
*                                                                           *
*     INTEGER                                                               *
*                                                                           *
*        NUMPEAK            # OF PEAKS CONSIDERED                         *
*        LU                 OUTPUT LU #                                    *
*        DATE               TODAYS DATE AND TIME                           *
*        ORDER              THE PREDICTED ORDER OF ELUTION                 *
*        PEN1PT             NUMBER OF POINTS FOR PEN 1                     *
*        PEN2PT             NUMBER OF POINTS FOR PEN 2                     *
*        PEN3PT             NUMBER OF POINTS FOR PEN 3                     *
*        PEN4PT             NUMBER OF POINTS FOR PEN 4                     *
*        ISAMPLE            INTEGER REPRESENTATION OF SAMPLE NAME          *
*        ICOLUMN            INTEGER REPRESENTATION OF COLUMN NAME          *
*        I_MEOH             INTEGER REPRESENTATION OF MEOH VALUE           *
*        I_ACN              INTEGER REPRESENTATION OF ACN VALUE            *
*        I_THF              INTEGER REPRESENTATION OF THF VALUE            *
*        ISCALE             FRACTION OF RESOLUTION AT BEST COMP            *
*        PAGE               COUNTER FOR ITEMS ON A PAGE                    *
*        PLOT               HOLDS DECISION TO PLOT LINES OF RESOL          *
*        XARRAY             ARRAY OF POINTS TO PLOT                        *
*        YARRAY             ARRAY OF POINTS TO PLOT                        *
*        PARRAY             ARRAY OF POINTS TO PLOT                        *
*        QARRAY             ARRAY OF POINTS TO PLOT                        *
*                                                                           *
*     REAL                                                                  *
*                                                                           *
*        COF                CHROMATOGRAPHIC OPTIMIZATION FUNCTION          *
*        VOIDRT             RETENTION TIME OF THE SOLVENT FRONT            *
*        WIDTH              PEAK WIDTH IN SECONDS                          *
*        KPRIME             K' CAPACITY FACTOR                             *
*        PEAKRT             PEAK RETENTION TIME IN MINUTES                 *
*        RESWANT            RESOLUTION DESIRED                             *
*        RESOLUTION         RESOLUTION BETWEEN PEAKS                       *
*        MINRES             MINIMUM RESOLUTION FOR POINTS IN TRIANGLE      *
*        BESTRES            WORST RESOLUTION AT BEST CONDITIONS            *
*        TIME               PREDICTED RETENTION TIMES                      *
*        BESTX1             AMOUNT OF MEOH AT BEST COMP                    *
*        BESTX2             AMOUNT OF ACN AT BEST COMP                     *
*        BESTX3             AMOUNT OF THF AT BEST COMT                     *
*        I9,J9,L9,M9,N9,O9  ARRAYS OF TRIANGLE LINES                       *
*        G1                 OFFSET FOR PLOTTER                             *
*        G2                 MAXIMUM VALUE FOR PLOTTER                      *
*        PEN1X              X COORDINATES FOR PEN 1                        *
*        PEN1Y              Y COORDINATES FOR PEN 1                        *
*        PEN2X              X COORDINATES FOR PEN 2                        *
*        PEN2Y              Y COORDINATES FOR PEN 2                        *
*        PEN3X              X COORDINATES FOR PEN 3                        *
*        PEN3Y              Y COORDINATES FOR PEN 3                        *
*        PEN4X              X COORDINATES FOR PEN 4                        *
*        PEN4Y              Y COORDINATES FOR PEN 4                        *
*        WIDE               MAXIMUM WINDOW WIDTH                           *
*        HEIGHT             MAXIMUM WINDOW HEIGHT                          *
*        VMAX               VIRTUAL MAXIMUM                                *
*        VMIN               VIRTUAL MINIMUM                                *
*        BETA1-BETA7        CHROMATOGRAPHIC BETA VALUES 1-7                *
*        Y                  RESOLUTION AT A SPECIFIC COMPOSITION           *
*        FLOW               SOLVENT FLOW RATE (ml/min)                     *
```

```
*        GO                  RERUN FLAG                                    *
*        CHOSX1-CHOSX3       SELECTED SOLVENT COMPOSITION                  *
*        SCALE               FRACTION OF THE BEST RESOLUTION               *
*                                                                          *
*                                                                          *
*     CHARACTER                                                            *
*                                                                          *
*        PEAKNAME(35)*15     NAME OF THE PEAK                              *
*        SOLV(7)*9           NAME OF SOLVENTS                              *
*        QUEST*1             ANSWERS TO QUESTIONS                          *
*        FF*1                FORM FEED                                     *
*        ESC*1               ESCAPE CODE                                   *
*        FILE1*14            NAME OF DISC FILE HOLDING DATA                *
*        C_MEOH*4            CHARACTER REPRESENTATION OF MEOH VALUE        *
*        C_ACN*4             CHARACTER REPRESENTATION OF ACN VALUE         *
*        C_THF*4             CHARACTER REPRESENTATION OF THF VALUE         *
*        CSAMPLE*            CHARACTER REPRESENTATION OF SAMPLE NAME       *
*        CCOLUMN*16          CHARACTER REPRESENTATION OF COLUMN NAME       *
*        CSCALE*6            CHARACTER REPRESENTATION OF SCALE             *
*                                                                          *
****************************************************************************
*                          INITIALIZATION                                  *
*                                                                          *
      PROGRAM LCMAIN
      COMMON /ONE/NUMPEAK,DATE,BESTX1,BESTX2,BESTX3,PEAKNAME
      COMMON /TWO/BESTRES,MINRES,WIDTH,KPRIME,PEAKRT,VOIDRT
      COMMON /THREE/RESOLUTION
      COMMON /FOUR/PEN1X,PEN1Y,PEN2X,PEN2Y,PEN3X,PEN3Y,PEN4X,PEN4Y
      COMMON /FIVE/PEN1PT,PEN2PT,PEN3PT,PEN4PT,ISAMPLE,ICOLUMN,
     1 I_MEOH,I_THF,I_ACN,ISCALE
      COMMON /SIX/XARRAY,YARRAY,PARRAY,QARRAY
      COMMON ESC,FF,LU
      INTEGER NUMPEAK,LU,DATE(15),ORDER(35),CONTRL,IERR,PEN1PT,
     1 PEN2PT,PEN3PT,PEN4PT,ISAMPLE(8),ICOLUMN(8),I_MEOH(2),I_THF(2),
     1 I_ACN(2),ISCALE(3),PAGE,PLOT,XARRAY(101),YARRAY(101),
     1 PARRAY(101),QARRAY(101)
      REAL COF(7),VOIDRT(7),WIDTH(7,35),KPRIME(7,35),PEAKRT(7,35),
     1 RESWANT,RESOLUTION(7,35,35),MINRES(0:50,0:50),BESTRES,TIME(35),
     1 BESTX1,BESTX2,BESTX3,XB(0:10),YB(0:10),XL(0:10),YL(0:10),
     1 XR(0:10),YR(0:10),PEN1X(1300),PEN1Y(1300),PEN2X(1000),
     1 PEN2Y(1000),PEN3X(1000),PEN3Y(1000),PEN4X(1000),PEN4Y(1000),
     1 WIDE,HEIGHT,VMAX,VMIN
      CHARACTER PEAKNAME(35)*15,SOLV(7)*9,FILE1*14,C_MEOH*4,C_ACN*4,
     1 C_THF*4,CSAMPLE*16,CCOLUMN*16,CSCALE*6
      CHARACTER *1 ESC,FF,QUEST
      DIMENSION LUBUF(275)
      EQUIVALENCE (C_MEOH,I_MEOH),(C_THF,I_THF),(C_ACN,I_ACN),
     1 (CSAMPLE,ISAMPLE),(CCOLUMN,ICOLUMN),(CSCALE,ISCALE)
      DATA SOLV(1),SOLV(2),SOLV(3)/'MEOH','ACN','THF'/
      DATA SOLV(4),SOLV(5)/'MEOH&ACN','MEOH&THF'/
      DATA SOLV(6),SOLV(7)/'ACN&THF','ALL THREE'/
      ESC=CHAR(27)
      FF=CHAR(12)
      PEN1PT=0
      PEN2PT=0
      PEN3PT=0
      PEN4PT=0
C     CHANGE THE FILE TO FIT YOUR SYSTEM !
      FILE1(7:)=':JC:3:9'      ! PREPARE FILE TO BE ON LU JC,TYPE 3
      CALL LGBUF(LUBUF,275)
  100 WRITE (1,290) ESC,ESC    ! CLEAR SCREEN AND PRINT QUESTION
```

```
      READ (1,294) ICOLUMN
      WRITE(1,'(" ENTER THE SAMPLE NAME:  _")')
      READ (1,294) ISAMPLE
      WRITE(1,'(" DO YOU WANT TO USE AN OLD DATA FILE?  _")');
      READ (1,391) QUEST
      IF (QUEST.NE.'Y') THEN
         WRITE (1,291)
         READ (1,293) FILE1(:6)
         OPEN (333,FILE=FILE1,IOSTAT=IOS1,ERR=910,STATUS='NEW')
      ELSE
         WRITE (1,292)
         READ (1,293) FILE1(:6)
         OPEN (333,FILE=FILE1,IOSTAT=IOS1,ERR=910,STATUS='OLD')
         REWIND (333)
         READ (333) PEAKNAME
         DO 105 I=1,7
            READ (333) VOIDRT(I),(PEAKRT(I,J),WIDTH(I,J),J=1,35)
105      CONTINUE
         WRITE (1,289)
         READ *,NUMPEAK
         IF (NUMPEAK.EQ.0) STOP
         GOTO 225
      ENDIF
*
****   GET PEAK DATA
*
200   WRITE (1,289)
      READ *,NUMPEAK
      IF (NUMPEAK.EQ.0) STOP
      IF (NUMPEAK.LT.2.OR.NUMPEAK.GT.35) GOTO 200
      DO 220 I=1,7
         WRITE (1,280) SOLV(I)
         READ *,VOIDRT(I)
         IF (VOIDRT(I).EQ.0) STOP
         IF (I.LT.2) THEN
           WRITE (1,281)
           DO 205 J=1,NUMPEAK
              WRITE (1,282) J
              READ *,PEAKRT(I,J),WIDTH(I,J),PEAKNAME(J)
205        CONTINUE
         ELSE
210        WRITE (1,283)
           DO 215 J=1,NUMPEAK
              WRITE (1,284) PEAKNAME(J)
              READ *,PEAKRT(I,J),WIDTH(I,J)
215        CONTINUE
         ENDIF
220   CONTINUE
*
*****    PRINT INPUT
*
225   WRITE (1,285) VOIDRT
      DO 230 I=1,NUMPEAK
         WRITE (1,286) I,PEAKNAME(I),(PEAKRT(J,I),J=1,7)
         WRITE (1,287) (WIDTH (J,I),J=1,7)
230   CONTINUE
      WRITE (1,288)
280   FORMAT (/,'ENTER THE RETENTION TIME (MIN) FOR SOLVENT  ',A9,
     1'  <0=EXIT>')
281   FORMAT (/,'ENTER THE RETENTION TIME (MIN), PEAK WIDTH (SEC),',
     1' PEAK NAME',/,'PEAK #  RT   WIDTH   NAME')
```

```
184   282  FORMAT (T2,I2,3X," _")
185   283  FORMAT (/,'ENTER RETENTION TIME (MIN), AND PEAK WIDTH (SEC)',/,
186       1'   PEAK          RT   WIDTH')
187   284  FORMAT (T2,A15,1X," _")
188   285  FORMAT (/,T48,'ACN& ',T57,'THF&',T66,'ACN&',T74,'MEOH&',/,T21,
189       1'MEOH     ACN      THF      MEOH     MEOH     THF     ACN&THF',/,
190       1T22,'1',T31,'2',T40,'3',T49,'4',T58,'5',T67,'6',T76,'7',/,T19,
191       1'-------------------------------------------------------',/,
192       1T5,'SOLVENT FRONT',T21,F5.2,6F9.2,/)
193   286  FORMAT (I3,X1,A15,T21,F5.2,6F9.2)
194   287  FORMAT (T22,'(',I3,')',T31,'(',I3,')',T40,'(',I3,')',T49,,'(',I3,
195       1')',T58,'(',I3,')',T67,'(',I3,')',T76,'(',I3,')')
196   288  FORMAT (T19,'-----------------------------------------------',
197       1'------------')
198   289  FORMAT ('ENTER THE NUMBER OF PEAKS PER SOLVENT. (2-35)  <0=EXIT>')
199   290   FORMAT (A1,'H',A1,'J',//,T30,'HPLC OPTIMIZATION',//,
200       1' ENTER THE COLUMN NAME:  _')
201   291  FORMAT (' ENTER THE NAME OF THE NEW FILE. _')
202   292  FORMAT (' ENTER THE NAME OF THE OLD FILE. _')
203   293  FORMAT (A6)
204   294  FORMAT (8A2)
205   295  FORMAT (A1,'H',A1,'J')
206  *                                                                    *
207  ********************   CHANGE SECTION  ***********************************
208  *                                                                    *
209   300  WRITE (1,'(" ARE THERE ANY CHANGES? _")')
210        READ (1,391) QUEST
211        IF (QUEST.NE.'Y') GOTO 320
212        WRITE (1,'(" DO YOU WANT TO CHANGE A NAME? _")')
213        READ (1,391) QUEST
214        IF (QUEST.NE.'Y') GOTO 305
215        WRITE (1,'(" ENTER THE PEAK #  _")')
216        READ *,I
217        WRITE (1,394) I,PEAKNAME(I)
218        READ *,PEAKNAME(I)
219        GOTO 315
220   305  WRITE (1,'(" WHICH SOLVENT? _")')
221        READ *,I
222   310  WRITE (1,'("WHAT DO YOU WANT CHANGED? (VOIDRT,PEAKRT,OR WIDTH)")')
223        READ (1,391) QUEST
224        IF (QUEST.EQ.'V') THEN
225           WRITE (1,385) VOIDRT(I)
226           READ *,VOIDRT(I)
227        ELSEIF (QUEST.EQ.'P') THEN
228           WRITE (1,'(" WHICH PEAK # ? _")')
229           READ *,J
230           WRITE (1,386) PEAKNAME(J),PEAKRT(I,J)
231           READ *,PEAKRT(I,J)
232        ELSEIF (QUEST.EQ.'W') THEN
233           WRITE (1,'(" WHICH PEAK # ? _")')
234           READ *,J
235           WRITE (1,387) PEAKNAME(J),WIDTH(I,J)
236           READ *,WIDTH (I,J)
237        ELSE
238        GOTO310
239        ENDIF
240        WRITE (1,'(" ANY OTHER CHANGES FOR THIS SOLVENT? _")')
241        READ (1,391) QUEST
242        IF (QUEST.EQ.'Y') GOTO 310
243   315  WRITE (1,'("ANY OTHER CHANGES? _")')
244        READ (1,391) QUEST
```

```
      IF (QUEST.EQ.'Y') GOTO 305
      GOTO 225
***     WRITE THE DATA TO THE DISC FILE
 320  REWIND (333)
      WRITE (333) PEAKNAME
      DO 325 I= 1,7
          WRITE (333) VOIDRT(I),(PEAKRT(I,J),WIDTH(I,J),J=1,35)
 325  CONTINUE
      CLOSE (333)
      WRITE (1,'("DO YOU WANT TO ANALYSE THE ENTIRE LIST? <Y/N> _")')
      READ (1,391) QUEST
      IF (QUEST.EQ.'Y') GOTO 360
      WRITE (1,'("HOW MANY PEAKS DO YOU WANT TO ANALYSE? _")')
      READ *,NUMPEAK
      DO 335 I=1,NUMPEAK
         WRITE (1,'("ENTER A PEAK NUMBER. _")')
 330     READ *,ORDER(I)
         WRITE (1,395) ORDER(I),PEAKNAME(ORDER(I))
         READ (1,391) QUEST
         IF (QUEST.NE.'Y') THEN
            WRITE (1,'("RE-ENTER THE PEAK #. _")')
            GOTO 330
         ENDIF
 335  CONTINUE
      DO 345 I=1,NUMPEAK-1
         DO 340 J=I+1,NUMPEAK
            IF (ORDER(J).LT.ORDER(I)) THEN
               ORD1=ORDER(I)
               ORDER(I)=ORDER(J)
               ORDER(J)=ORD1
            ENDIF
 340     CONTINUE
 345  CONTINUE
      DO 355 I=1,NUMPEAK
         PEAKNAME(I)=PEAKNAME(ORDER(I))
         DO 350 J=1,7
            PEAKRT(J,I)=PEAKRT(J,ORDER(I))
            WIDTH(J,I)=WIDTH(J,ORDER(I))
 350     CONTINUE
 355  CONTINUE
 360  DO 370 I=1,7
         VRT=VOIDRT(I)*60
         DO 365 J=1,NUMPEAK
              RT=PEAKRT(I,J)*60
              KPRIME(I,J)=(RT-VRT)/VRT
 365     CONTINUE
 370  CONTINUE
 375  WRITE (1,388)
      READ *,LU
C     CHANGE THE LU NUMBERS TO FIT YOUR SYSTEM
      IF (LU.EQ.6) WRITE (LU,389)    ! FORM FEED LINE PRINTER
      IF (LU.EQ.7.OR.LU.EQ.53) WRITE (LU,*) FF   ! FF 9871 OR 9876
      IF (LU.NE.1.AND.LU.NE.6.AND.LU.NE.7.AND.LU.NE.53) GOTO 375
      CALL FTIME(DATE)
      WRITE (LU,390)                  ! SKIP 3 LINES
      WRITE (LU,392) DATE,CCOLUMN,CSAMPLE
      WRITE (LU,285) VOIDRT
      DO 380 I=1,NUMPEAK
         WRITE (LU,286) I,PEAKNAME(I),(PEAKRT(J,I),J=1,7)
         WRITE (LU,287) (WIDTH(J,I),J=1,7)
 380  CONTINUE
```

```
      WRITE (LU,288)
 385  FORMAT (" VOIDRT= ",F5.2,"    NEW VALUE IS TO BE ","  _")
 386  FORMAT (T2,A15," RETENTION TIME = ",F7.2,"   NEW VALUE ","  _")
 387  FORMAT (T2,A15," PEAK WIDTH = ",F7.2,"       NEW VALUE ","  _")
C     CHANGE THE LU NUMBERS TO FIT YOUR SYSTEM
 388  FORMAT (/," WHERE DO YOU WANT THE OUTPUT ?",/,T10,"1 = THIS TERM",
     1"INAL ",/,T10,"6 = THE LINE PRINTER",/,T10,"7 = THE DAISY WHEEL ",
     1"PRINTER",/,T10,"53= THE THERMAL PRINTER")
 389  FORMAT ("1")
 390  FORMAT (/,/)
 391  FORMAT (A1)
 392  FORMAT (T30,'HPLC OPTIMIZATION',//,T23,15A2,//,T34,'INPUT DATA',/,
     1T20,'COLUMN :',A16,T45,'SAMPLE :',A16,//,T25,'(DATA IS CORRECTED',
     1' TO 1.00 ml/min)')
 393  FORMAT (A15)
 394  FORMAT (' PEAK ',I2,' IS CURRENTLY ',A15,/,' ENTER THE NEW ',
     1'NAME     ')
 395  FORMAT (7,'PEAK # ',I2,' IS CURRENTLY ',A15,' OK? <Y/N> _')
*
************************** CALCULATE RESOLUTION **********************
*
      DO 410 I=1,7
         DO 405 J=1,NUMPEAK-1
            DO 400 K=J+1,NUMPEAK
            RESOLUTION (I,J,K)=(PEAKRT(I,K)*60.-PEAKRT(I,J)*60.)/
     1       ((WIDTH(I,K)+WIDTH(I,J))*0.5)
 400        CONTINUE
 405     CONTINUE
 410  CONTINUE
      WRITE (1,'(" DO YOU WANT TO CALCULATE THE COF ? <Y/N> _")')
      READ (1,391) QUEST
      IF (QUEST.EQ.'Y') THEN
 415    WRITE (1,'(" ENTER THE DESIRED RESOLUTION. _")')
        READ *,RESWANT
        IF (RESWANT.LT.0) GOTO 415
        DO 430 I=1,7
           COF(I)=0
           DO 425 J=1,NUMPEAK-1
              DO 420 K=J+1,NUMPEAK
                 Z=RESOLUTION(I,J,K)/RESWANT
                 IF (Z.LE.0) GOTO 420
                 COF(I)=COF(I)+ALOG(Z)
 420          CONTINUE
 425       CONTINUE
 430    CONTINUE
*
***   OUTPUT
*
       DO 450 I=1,7
C      CHANGE THE LU NUMBERS TO FIT YOUR SYSTEM
          IF (LU.EQ.6) WRITE (LU,389)  ! FORM FEED LINE PRINTER
          IF (LU.EQ.7.OR.LU.EQ.53) WRITE (LU,*) FF  ! FF 9871 OR 9876
          WRITE (LU,490) SOLV(I),VOIDRT(I)
          DO 435 J=1,NUMPEAK
             WRITE (LU,491) PEAKNAME(J),PEAKRT(I,J),WIDTH(I,J),
     1         KPRIME(I,J)
 435      CONTINUE
          WRITE (LU,492)
          DO 445 J=1,NUMPEAK-1
             DO 440 K=J+1,NUMPEAK
                I3=INDEX(PEAKNAME(J),'  ')
```

```
367                 IF (I3.GT.15.OR.I3.LT.1) I3=15
368                 WRITE (LU,493) PEAKNAME(J)(:I3),PEAKNAME(K),
369        1            RESOLUTION(I,J,K)
370   440        CONTINUE
371   445      CONTINUE
372            WRITE (LU,494) SOLV(I),COF(I)
373   450    CONTINUE
374          ENDIF
375   490    FORMAT (//,T5,'TIME ZERO FOR SOLVENT ',A9,' IS',F7.2,
376         1' MIN.',/,/,' INGREDIENT',T20,'RETENTION TIME',T37,'BAND WIDTH',
377         1T50,'CAPACITY',/)
378   491    FORMAT (T2,A15,T25,F5.2,T40,I3,T51,F6.2)
379   492    FORMAT (//,T8,' FOR PEAKS',T35,'RESOLUTION',/)
380   493    FORMAT (T2,R15,'- ',A15,T36,F8.3)
381   494    FORMAT (//,' CHROMATOGRAPHIC OPTIMIZATION FUNCTION (COF) FOR ',
382         1A9,' IS',F9.4)
383  *                                                                      *
384  ************************************************************************
385  *                        CALLS TO SUBROUTINES                          *
386   500    GO=0
387   505    CALL LCSORT (GO)
388          WRITE (1,'("DO YOU WANT A PLOT OF THE RESOLUTION POINTS? _")')
389          READ (1,391) QUEST
390          IF (QUEST.EQ.'Y') CALL LCPOINT
391          WRITE (1,'("DO YOU WANT A PLOT OF THE RESOLUTION LINES? _")')
392          READ (1,391) QUEST
393          IF (QUEST.EQ.'Y') CALL LCLINE
394          WRITE (1,'("DO YOU WANT TO CALC FOR A DIFFERENT SOLVENT? _")')
395          READ (1,391) QUEST
396          GO=1
397          IF (QUEST.EQ.'Y') GOTO 505
398          WRITE (1,'(" THE END !")')
399  C       CHANGE THE LU NUMBERS TO FIT YOUR SYSTEM
400          IF (LU.EQ.6) WRITE (LU,389)    ! FORM FEED LINE PRINTER
401          IF (LU.EQ.7.OR.LU.EQ.53) WRITE (LU,*) FF   ! FF 9871 OR 9876
402          STOP
403  *                                                                      *
404  ************************** ERROR SECTION ********************************
405  *                                                                      *
406   910    WRITE (1,980) IOS1
407   980    FORMAT (//,'ERROR IN OPEN STATEMENT.  IOSTAT = ',I4)
408          END
```

```
*                                                                      *
************************  BEST SEPARATION SECTION  ************************
*                                                                      *
$EMA /TWO/,/THREE/,/FOUR/,/SIX/
      SUBROUTINE LCSORT (GO)
      COMMON /ONE/NUMPEAK,DATE,BESTX1,BESTX2,BESTX3,PEAKNAME
      COMMON /TWO/BESTRES,MINRES,WIDTH,KPRIME,PEAKRT,VOIDRT
      COMMON /THREE/RESOLUTION
      COMMON /FIVE/PEN1PT,PEN2PT,PEN3PT,PEN4PT,ISAMPLE,ICOLUMN,
     1 I_MEOH,I_THF,I_ACN,ISCALE
      COMMON ESC,FF,LU
      INTEGER NUMPEAK,LU,DATE(15),ORDER(35),CONTRL,IERR,PEN1PT,
     1 PEN2PT,PEN3PT,PEN4PT,ISAMPLE(6),ICOLUMN(8),I_MEOH(2),I_THF(2),
     1 I_ACN(2),ISCALE(3),PAGE,PLOT
      REAL VOIDRT(7),WIDTH(7,35),KPRIME(7,35),PEAKRT(7,35),
     1 RESOLUTION(7,35,35),MINRES(0:50,0:50),BESTRES,TIME(35),
     1 BESTX1,BESTX2,BESTX3
      CHARACTER PEAKNAME(35)*15,FILE1*14,C_MEOH*4,C_ACN*4,
     1 C_THF*4,CSAMPLE*16,CCOLUMN*16,CSCALE*6
      CHARACTER *1 ESC,FF,QUEST
      EQUIVALENCE (C_MEOH,I_MEOH),(C_THF,I_THF),(C_ACN,I_ACN),
     1 (CSAMPLE,ISAMPLE),(CCOLUMN,ICOLUMN),(CSCALE,ISCALE)
      IF (GO.GT.0) GOTO 145
100   DO 110 I=0,50
         DO 105 J=0,50-I
            MINRES(I,J)=1.0E38
105      CONTINUE
110   CONTINUE
      WRITE (1,388) ESC,ESC      ! REVERSE VIDIO AND PRINT "WORKING"
      DO 130 I=1,NUMPEAK-1
         IF (I.GT.1) WRITE (1,389) ESC,I,ESC  ! REVERSE VIDIO AGAIN
         DO 125 J=I+1,NUMPEAK
            BETA1 = RESOLUTION (1,I,J)
            BETA2 = RESOLUTION (2,I,J)
            BETA3 = RESOLUTION (3,I,J)
            BETA4 = 4.0*RESOLUTION (4,I,J) - 2.0*(BETA1+BETA2)
            BETA5 = 4.0*RESOLUTION (5,I,J) - 2.0*(BETA1+BETA3)
            BETA6 = 4.0*RESOLUTION (6,I,J) - 2.0*(BETA2+BETA3)
            BETA7 = 27.0*RESOLUTION(7,I,J) - 12.0*(RESOLUTION(4,I,J) +
     1     RESOLUTION(5,I,J)+RESOLUTION(6,I,J))+3.0*(BETA1+BETA2+BETA3)
            DO 120 I1=0,100,2
               DO 115 J1=0,100-I1,2
                  X1=I1/100.
                  X2=J1/100.
                  X3=1.0-X1-X2
                  Y=BETA1*X1+BETA2*X2+BETA3*X3+BETA4*X1*X2+BETA5*X1*X3+
     1              BETA6*X2*X3+BETA7*X1*X2*X3
                  Y=ABS(Y)
                  I2=I1/2
                  J2=J1/2
                  IF (Y.LE.MINRES(I2,J2)) MINRES(I2,J2)=Y
115            CONTINUE
120         CONTINUE
125      CONTINUE
130   CONTINUE
***   SELECT THE BEST COMPOSITION AND ITS WORST RESOLUTION
      WRITE (1,380) ESC,ESC                ! CLEAR THE SCREEN
      BESTRES=0
      DO 140 I=0,50
         DO 135 J=0,50-I
            IF (MINRES(I,J).GT.BESTRES) THEN
```

```
                BESTRES=MINRES(I,J)
                BESTX1=I*2.0
                BESTX2=J*2.0
                BESTX3=100.-BESTX1-BESTX2
              ENDIF
  135       CONTINUE
  140     CONTINUE
*
***************  PRINT BEST SEPARATION  **********************
*
C       CHANGE THE LU NUMBERS TO FIT YOUR SYSTEM
  145   IF (LU.EQ.6) WRITE (LU,381)       ! FORM FEED LINE PRINTER
        IF (LU.EQ.7.OR.LU.EQ.53) WRITE (LU,*) FF   ! FF 9871 OR 9876
        WRITE (LU,382)                    ! SKIP 3 LINES
        WRITE (LU,385) DATE,CCOLUMN,CSAMPLE,BESTX1,BESTX2,BESTX3,BESTRES
*
***************  PREDICT ORDER OF ELUTION  *******************
*
        CHOSX1=BESTX1
        CHOSX2=BESTX2
        CHOSX3=BESTX3
        RES=BESTRES
        WRITE (1,'("WHAT FLOW RATE ARE YOU INTERESTED IN? _")')
        READ *,FLOW
        WRITE (1,'("DO YOU WANT TO CHOSE YOUR OWN COMPOSITION? _")')
        READ (1,383) QUEST
        IF (QUEST.EQ.'Y') THEN
        WRITE (1,385) DATE,CCOLUMN,CSAMPLE,BESTX1,BESTX2,BESTX3,BESTRES
        WRITE (1,'("ENTER COMPOSITION YOU WANT TO CALC RES TIMES FOR")')
        READ *,CHOSX1,CHOSX2,CHOSX3
        I=INT(CHOSX1/2.0)
        J=INT(CHOSX2/2.0)
        RES=MINRES(I,J)
        IF (LU.EQ.6) WRITE (LU,381)       ! FORM FEED LINE PRINTER
        IF (LU.EQ.7.OR.LU.EQ.53) WRITE (LU,*) FF   ! FF 9871 OR 9876
        WRITE (LU,384) DATE,CCOLUMN,CSAMPLE,CHOSX1,CHOSX2,CHOSX3,RES
        ENDIF
        DO 200 I=1,NUMPEAK
            ORDER(I)=I
  200   CONTINUE
        DO 205 I=1,NUMPEAK
           BETA1 = KPRIME(1,I)
           BETA2 = KPRIME(2,I)
           BETA3 = KPRIME(3,I)
           BETA4 = 4.0*KPRIME(4,I)-2.0*(BETA1+BETA2)
           BETA5 = 4.0*KPRIME(5,I)-2.0*(BETA1+BETA3)
           BETA6 = 4.0*KPRIME(6,I)-2.0*(BETA2+BETA3)
           BETA7 = 27.0*KPRIME(7,I)-12.0*(KPRIME(4,I)+KPRIME(5,I)+
     1      KPRIME(6,I))+3.0*(BETA1+BETA2+BETA3)
           X1=CHOSX1/100.
           X2=CHOSX2/100.
           X3=CHOSX3/100.
           Y=(BETA1*X1+BETA2*X2+BETA3*X3+BETA4*X1*X2+BETA5*X1*X3+
     1      BETA6*X2*X3+BETA7*X1*X2*X3)
           TIME(I)=VOIDRT(1)*(1+Y)
  205   CONTINUE
*
*****************  SELECT ORDER  ************
*
        DO 215 I=1,NUMPEAK-1
           DO 210 J=I+1,NUMPEAK
```

```
531               IF (TIME(J).LT.TIME(I)) THEN
532                  ORD1=ORDER(I)
533                  ORDER(I)=ORDER(J)
534                  ORDER(J)=ORD1
535                  T1=TIME(I)
536                  TIME(I)=TIME(J)
537                  TIME(J)=T1
538               ENDIF
539  210       CONTINUE
540  215  CONTINUE
541       WRITE (LU,386) FLOW
542       DO 220 I=1,NUMPEAK
543          J=ORDER(I)
544          WRITE (LU,387)I,PEAKNAME(J),TIME(I).TIME(I)/FLOW
545  220  CONTINUE
546 C     CHANGE THE LU NUMBERS TO FIT YOUR SYSTEM
547       IF (LU.EQ.6) WRITE (LU,381)      ! FORM FEED LINE PRINTER
548       IF (LU.EQ.7.OR.LU.EQ.53) WRITE (LU,*) FF  ! FF 9871 OR 9876
549  380  FORMAT (A1,'H',A1,'J')
550  381  FORMAT ("1")
551  382  FORMAT (/,/)
552  383  FORMAT (A1)
553  384  FORMAT (T30,'HPLC OPTIMIZATION',/,T23,15A2,//,T32,
554       1'DATA ANALYSIS',/,T20,'COLUMN :',A16,T45,'SAMPLE :',A16,//,T25,
555       1'THE SELECTED COMPOSITION IS :',/,T21,'MEOH',T36,
556       1'ACN',T52,'THF',/,T21,I3,' %',T35,I3,' %',T51,I3,' %',//,T15,
557       1'THE WORST RESOLUTION AT THIS POINT IS ',F7.3,//)
558  385  FORMAT (T30,'HPLC OPTIMIZATION',/,T23,15A2,//,T32,
559       1'DATA ANALYSIS',/,T20,'COLUMN :',A16,T45,'SAMPLE :',A16,//,T25,
560       1'THE BEST COMPOSITION IS :',/,T21,'MEOH',T36,'ACN',T52,'THF',/,
561       1T21,I3,' %',T35,I3,' %',T51,I3,' %',//,T15,'THE WORST RESOLUTION',
562       1' AT THIS POINT IS ',F7.3,//)
563  386  FORMAT (//,T27,'PREDICTED ORDER OF ELUTION',//,T40,'RELATIVE ',
564       1'RETENTION TIME',/,T24,'INGREDIENT',T40,'1.00 ml/min ',
565       1F5.2,' ml/min',/)
566  387  FORMAT (T16,I2,T24,A15,T42,F6.2,T55,F6.2)
567  388  FORMAT (//,A1,'&dC WORKING!  1',A1,'&@')
568  389  FORMAT (A1,'&dC WORKING! ',I3,A1,'&@')
569       RETURN
570       END
```

```
*                                                                      *
********************** SUBROUTINE TO PLOT POINT GRAPH ******************
*                                                                      *
$EMA /TWO/,/THREE/,/FOUR/,/SIX/
      SUBROUTINE LCPOINT
      COMMON /ONE/NUMPEAK,DATE,BESTX1,BESTX2,BESTX3,PEAKNAME
      COMMON /TWO/BESTRES,MINRES,WIDTH,KPRIME,PEAKRT,VOIDRT
      COMMON /FOUR/PEN1X,PEN1Y,PEN2X,PEN2Y,PEN3X,PEN3Y,PEN4X,PEN4Y
      COMMON /FIVE/PEN1PT,PEN2PT,PEN3PT,PEN4PT,ISAMPLE,ICOLUMN,
     1 I_MEOH,I_THF,I_ACN,ISCALE
      COMMON ESC,FF,LU
      INTEGER NUMPEAK,DATE(15),CONTRL,IERR,PEN1PT,
     1 PEN2PT,PEN3PT,PEN4PT,ISAMPLE(8),ICOLUMN(8),I_MEOH(2),I_THF(2),
     1 I_ACN(2),ISCALE(3),PAGE,PLOT
      REAL WIDTH(7,35),KPRIME(7,35),PEAKRT(7,35),
     1 RESWANT,MINRES(0:50,0:50),BESTRES,
     1 BESTX1,BESTX2,BESTX3,XB(0:10),YB(0:10),XL(0:10),YL(0:10),
     1 XR(0:10),YR(0:10),PEN1X(1300),PEN1Y(1300),PEN2X(1000),
     1 PEN2Y(1000),PEN3X(1000),PEN3Y(1000),PEN4X(1000),PEN4Y(1000),
     1 WIDE,HEIGHT,VMAX,VMIN
      CHARACTER C_MEOH*4,C_ACN*4,
     1 C_THF*4,CSAMPLE*16,CCOLUMN*16,CSCALE*6
      CHARACTER *1 ESC,FF,QUEST
      EQUIVALENCE (C_MEOH,I_MEOH),(C_THF,I_THF),(C_ACN,I_ACN),
     1 (CSAMPLE,ISAMPLE),(CCOLUMN,ICOLUMN),(CSCALE,ISCALE)
*                                                                      *
************************************************************************
*                        PLOT MINIMUM RESOLUTION                       *
      G1=20.
      G2=350.
      Y_INCR=G2*(SQRT(3.0)/2)/10.
      DO 500 I1=0,10
         F=I1
         XB(I1)=INT(G1+(Y_INCR*F)/(SQRT(3.0)/2))
         YB(I1)=INT(G1)
         XL(I1)=INT(G1+(Y_INCR*F)/(SQRT(3.0)/1))
         YL(I1)=INT(G1+(Y_INCR*F))
         XR(I1)=INT(G1+(Y_INCR*10+Y_INCR*F)/(SQRT(3.0)/1))
         YR(I1)=INT(G1+(Y_INCR*(10-I1)))
 500  CONTINUE
      WRITE(1,590) ESC,ESC          ! REVERSE VIDIO PRINT "PLOTTING"
*
****** SELECT PEN COLOR ***
*
      SCALE=BESTRES/4.0
      K=1
      L=1
      M=1
      N=1
      DO 510 I=0,50
         DO 505 J=0,50-I
            X1=I*2./100.
            X2=J*2./100.
            X3=1.0-X1-X2
            X=G1+(1.0-X3)*G2/2+(1.0*X2*G2/2)
            Y=G1+(X1*G2*SQRT(3.0)/2)
            RES=MINRES(I,J)
            IF (RES.LE.SCALE) THEN
               PEN1X(K)=X
               PEN1Y(K)=Y
               PEN1PT=K
```

```
632                K=K+1
633             ELSEIF (RES.LE.(SCALE*2.0)) THEN
634                PEN2X(L)=X
635                PEN2Y(L)=Y
636                PEN2PT=L
637                L=L+1
638             ELSEIF (RES.LE.(SCALE*3.0)) THEN
639                PEN3X(M)=X
640                PEN3Y(M)=Y
641                PEN3PT=M
642                M=M+1
643             ELSEIF (RES.LE.(SCALE*3.75)) THEN
644                PEN4X(N)=X
645                PEN4Y(N)=Y
646                PEN4PT=N
647                N=N+1
648             ENDIF
649  505     CONTINUE
650  510  CONTINUE
651  *
652  ******* PLOT TRIANGULAR GRAPH  (USES H-P DGL GRAPHICS PACKAGE)
653  *
654        CONTRL=0
655        CALL ZBEGN
656  C     CHANGE "54" TO FIT YOUR SYSTEM
657        CALL ZDINT (54,CONTRL,IERR)   ! INITIALIZE PLOTTER ON LU 54
658        VMIN=0.0
659        VMAX=1.0
660        WIDE =410          ! THE MAX X VALUE IN WORLD COORDINATES
661        HEIGHT=410         ! THE MAX Y VALUE IN WORLD COORDINATES
662        XLIM=225           ! THE MAX X DISTANCE IN MILLIMETERS
663        YLIM=225           ! THE MAX Y DISTANCE IN MILLIMETERS
664        CALL ZWIND (VMIN,WIDE ,VMIN,HEIGHT)
665        CALL ZDLIM (0,XLIM,0,YLIM,IERR)
666        CALL ZASPK (XLIM,YLIM)
667        CALL ZVIEW (VMIN,VMAX,VMIN,VMAX)
668        LM1=10/2
669        DO 520 N1=0,5
670           CALL ZMOVE (XL(N1),YL(N1))
671           CALL ZDRAW (XB(N1),YB(N1))
672           CALL ZDRAW (XR(N1),YR(N1))
673           IF (N1.LT.LM1) THEN
674              N2=10-N1
675              CALL ZDRAW (XL(N2),YL(N2))
676              CALL ZDRAW (XB(N2),YB(N2))
677              CALL ZDRAW (XR(N2),YR(N2))
678           ENDIF
679           CALL ZDRAW (XL(N1),YL(N1))
680  520  CONTINUE
681        CALL ZMCUR
682        CALL ZCSIZ (8.75,12.5)
683        CALL ZCOLR (1)
684        X=5
685        Y=5
686        CALL ZMOVE (X,Y)
687        CALL ZTEXT (3,3HTHF)
688        X=360
689        Y=5
690        CALL ZMOVE (X,Y)
691        CALL ZTEXT (3,3HACN)
692        X=180
```

```
      Y=335
      CALL ZMOVE (X,Y)
      CALL ZTEXT (4,4HMeOH)
      WRITE (C_MEOH,'(I4)') BESTX1
      WRITE (C_ACN,'(I4)') BESTX2
      WRITE (C_THF,'(I4)') BESTX3
      WRITE (CSCALE,'(F6.3)') SCALE
      X1=30
      X2=220
      X3=240
      X4=260
      X5=280
      X6=263
      X7=300
      X8=320
      X9=310
      X10=340
      X11=360
      X12=395
      CALL ZCOLR(1)
      CALL ZMOVE(X3,X11)
      CALL ZTEXT(18,18H HPLC OPTIMIZATION)
      CALL ZMOVE(X4,X10)
      CALL ZTEXT(14,14H DATA ANALYSIS)
      CALL ZMOVE(X3,X8)
      CALL ZCSIZ(5.5,9.0)
      CALL ZTEXT(30,DATE)
      CALL ZMOVE(X4,X7)
      CALL ZTEXT(9,9H COLUMN :)
      CALL ZMOVE(X9,X7)
      CALL ZTEXT(15,ICOLUMN)
      CALL ZMOVE(X4,X5)
      CALL ZTEXT(9,9H SAMPLE :)
      CALL ZMOVE(X9,X5)
      CALL ZTEXT(15,ISAMPLE)
      CALL ZMOVE(X4,X4)
      CALL ZTEXT(26,26H THE BEST COMPOSITION IS  )
      CALL ZMOVE(X4,X3)
      CALL ZTEXT(23,23H     MEOH     ACN     THF)
      CALL ZMOVE(X5,X2)
      CALL ZTEXT(4,I_MEOH)
      CALL ZTEXT(1,1H%)
      CALL ZMOVE(X8,X2)
      CALL ZTEXT(4,I_ACN)
      CALL ZTEXT(1,1H%)
      CALL ZMOVE(X11,X2)
      CALL ZTEXT(4,I_THF)
      CALL ZTEXT(1,1H%)
*
**********  PLOT WORST RESOLUTION POINTS  ***
*
      CALL ZCOLR(1)
      DO 535 I=1,PEN1PT
         WX=PEN1X(I)
         WY=PEN1Y(I)
         CALL ZMOVE(WX,WY)
         CALL ZMARK(8)
535   CONTINUE
      CALL ZMOVE(X1,X11)
      CALL ZMARK(8)
      CALL ZTEXT(15,15H  RESOLUTION < )
```

```
      CALL ZTEXT(6,ISCALE)
      CALL ZMCUR
      CALL ZCOLR(1)
      WRITE(CSCALE,'(F6.3)') SCALE*2
      DO 540 I=1,PEN2PT
         WX=PEN2X(I)
         WY=PEN2Y(I)
         CALL ZMOVE(WX,WY)
         CALL ZMARK(3)
540   CONTINUE
      CALL ZMOVE(X1,X10)
      CALL ZMARK(3)
      CALL ZTEXT(15,15H  RESOLUTION < )
      CALL ZTEXT(6,ISCALE)
      CALL ZMCUR
      CALL ZCOLR(2)
      WRITE(CSCALE,'(F6.3)') SCALE*3
      DO 545 I=1,PEN3PT
         WX=PEN3X(I)
         WY=PEN3Y(I)
         CALL ZMOVE(WX,WY)
         CALL ZMARK(6)
545   CONTINUE
      CALL ZMOVE(X1,X8)
      CALL ZMARK(6)
      CALL ZTEXT(15,15H  RESOLUTION < )
      CALL ZTEXT(6,ISCALE)
      CALL ZMCUR
      CALL ZCOLR(3)
      WRITE(CSCALE,'(F6.3)') SCALE*3.75
      DO 550 I=1,PEN4PT
         WX=PEN4X(I)
         WY=PEN4Y(I)
         CALL ZMOVE(WX,WY)
         CALL ZMARK(9)
550   CONTINUE
      CALL ZMOVE(X1,X7)
      CALL ZMARK(9)
      CALL ZTEXT(15,15H  RESOLUTION < )
      CALL ZTEXT(6,ISCALE)
      X=G1+(100-BESTX3)*G2/200+(BESTX2*G2/200)
      Y=G1+(BESTX1*G2*SQRT(3.0)/200)
      CALL ZCOLR(4)
      CALL ZMOVE(X,Y)
      CALL ZMARK(4)
      CALL ZMARK(2)
      WRITE (CSCALE,'(F6.3)') SCALE*4.0
      CALL ZMOVE(X1,X5)
      CALL ZMARK(4)
      CALL ZMARK(2)
      CALL ZTEXT(15,15H  RESOLUTION = )
      CALL ZTEXT(6,ISCALE)
      CALL ZMOVE(X12,X6)
      CALL ZMARK(4)
      CALL ZMARK(2)
      CALL ZMCUR
      CALL ZDEND
      CALL ZEND
      WRITE (1,591) ESC,ESC,ESC   ! CLEAR THE REVERSE VIDIO
590   FORMAT(A1,'&dC PLOTTING! PLOTTING! PLOTTING! ',A1,'&@')
591   FORMAT(A1,'A',A1,'J',A1,'B')
      RETURN
      END
```

```
817 *                                                                      *
818 ********************* SUBROUTINE TO PLOT LINES OF RESOLUTION ***********
819 *                                                                      *
820 $EMA /TWO/,/THREE/,/FOUR/,/SIX/
821       SUBROUTINE LCLINE
822       COMMON /ONE/NUMPEAK,DATE,BESTX1,BESTX2,BESTX3,PEAKNAME
823       COMMON /THREE/RESOLUTION
824       COMMON /FIVE/PEN1PT,PEN2PT,PEN3PT,PEN4PT,ISAMPLE,ICOLUMN,
825      1 I_MEOH,I_THF,I_ACN,ISCALE
826       COMMON /SIX/XARRAY,YARRAY,PARRAY,QARRAY
827       COMMON ESC,FF,LU
828       INTEGER NUMPEAK,DATE(15),PEN1PT,PEN2PT,PEN3PT,PEN4PT,
829      1 ISAMPLE(8),ICOLUMN(8),I_MEOH(2),I_THF(2),I_ACN(2),ISCALE(3),
830      1 PAGE,PLOT,XARRAY(101),YARRAY(101),PARRAY(101),QARRAY(101)
831       REAL RESWANT,RESOLUTION(7,35,35),
832      1 XB(0:10),YB(0:10),XL(0:10),YL(0:10),XR(0:10),YR(0:10)
833       CHARACTER PEAKNAME(35)*15,CSAMPLE*16,CCOLUMN*16,CSCALE*6
834       CHARACTER *1 ESC,FF,QUEST
835       EQUIVALENCE (C_MEOH,I_MEOH),(C_THF,I_THF),(C_ACN,I_ACN),
836      1 (CSAMPLE,ISAMPLE),(CCOLUMN,ICOLUMN),(CSCALE,ISCALE)
837 *                                                                      *
838 ************************************************************************
839 *                        PLOT LINES OF RESOLUTION                      *
840  600  WRITE (1,'(" WHAT IS THE MINIMUM RESOLUTION DESIRED? ")')
841       READ *,RESWANT
842       WRITE (1,870) RESWANT
843       PAGE=2
844       WRITE (1,887) ESC,ESC        ! CLEAR THE SCREEN
845       WRITE(1,888) DATE,CCOLUMN,CSAMPLE,ESC,ESC !PRINT HEADING ON 9876
846 *
847 ******* GET BETA VALUES
848 *
849       DO 750 I=1,NUMPEAK-1
850          DO 745 J=I+1,NUMPEAK
851             WRITE (1,886) ESC         ! TURN OFF GRAPHICS DISPLAY
852             BETA1 = RESOLUTION (1,I,J)
853             BETA2 = RESOLUTION (2,I,J)
854             BETA3 = RESOLUTION (3,I,J)
855             BETA4 = 4.0*RESOLUTION (4,I,J) - 2.0*(BETA1+BETA2)
856             BETA5 = 4.0*RESOLUTION (5,I,J) - 2.0*(BETA1+BETA3)
857             BETA6 = 4.0*RESOLUTION (6,I,J) - 2.0*(BETA2+BETA3)
858             BETA7 = 27.0*RESOLUTION(7,I,J) - 12.0*(RESOLUTION(4,I,J) +
859      1    RESOLUTION(5,I,J)+RESOLUTION(6,I,J))+3.0*(BETA1+BETA2+BETA3)
860 *
861 ********** CHECK FOR RESWANT, -RESWANT, AND 0
862 *
863             Y=0
864             PLOT=0
865             MARK=1
866             I3=INDEX(PEAKNAME(I),'  ')
867             IF (I3.GT.15.OR.I3.LT.1) I3=15
868 C     CLEAR THE SCREEN AND PRINT THE PEAK PAIR
869             WRITE (1,871) ESC,ESC,PEAKNAME(I)(:I3),PEAKNAME(J)
870             WRITE (1,872)Y
871             GOTO 620
872  610        IF (PLOT.EQ.1) GOTO 640
873             Y=RESWANT
874             WRITE (1,872)Y
875             MARK=2
876             GOTO 620
877  615        IF (PLOT.EQ.1) GOTO 640
```

```
878               Y=-RESWANT
879               WRITE (1,872)Y
880               MARK=3
881  *
882  *********  MAKES PLOT DECISION FOR A PEAK PAIR  **********
883  *
884   620         DO 635 IX=0,100,2
885                  X1=IX/100.
886                  C1=BETA3+(BETA1-BETA3+BETA5-BETA5*X1)*X1
887                  C2=BETA2-BETA3+BETA6+(BETA4-BETA5-BETA6+BETA7-
888        1            BETA7*X1)*X1
889                  C3=0-BETA6-BETA7*X1
890                  A=C3
891                  B=C2
892                  C=C1-Y
893                  D=B*B-4*A*C
894                  IF (D.LT.0) GOTO 635
895                  S=SQRT(D)
896                  R1=(0-B+S)/(2*A)
897                  R2=(0-B-S)/(2*A)
898                  IF (R1.LT.0.OR.R1.GT.1) GOTO 625
899                  Q1=X1+R1
900                  IF (Q1.GT.1) GOTO 625
901                  PLOT=1
902   625            IF (R2.LT.0.OR.R2.GT.1) GOTO 630
903                  Q2=X1+R2
904                  IF (Q2.GT.1) GOTO 630
905                  PLOT=2
906   630            IF (PLOT.EQ.1) GOTO (610,615,640) MARK
907   635         CONTINUE
908               GOTO (610,615,640) MARK
909   640         IF (PAGE.GT.1.AND.PLOT.EQ.1.AND.J.GT.2) THEN
910                  WRITE (1,873) ESC,ESC,ESC,ESC  ! FORM FEED FOR 9876
911                  PAGE=1
912               ELSEIF (PAGE.GT.3) THEN
913                  WRITE (1,873) ESC,ESC,ESC,ESC  ! FORM FEED FOR 9876
914                  PAGE=1
915               ENDIF
916               WRITE (53,874) PEAKNAME(I)(:13),PEAKNAME(J),
917        1      BETA1,BETA2,BETA3,BETA4,BETA5,BETA6,BETA7  ! OUTPUT TO 9876
918               WRITE (53,891)                             ! OUTPUT TO 9876
919               X1=0.0
920               X2=0.0
921               X3=1.0
922               Y=BETA1*X1+BETA2*X2+BETA3*X3+BETA4*X1*X2+BETA5*X1*X3+
923        1        BETA6*X2*X3+BETA7*X1*X2*X3
924               WRITE (53,875)X1*100.,X2*100.,X3*100.,Y    ! OUTPUT TO 9876
925               X1=0.0
926               X2=1.0
927               X3=0.0
928               Y=BETA1*X1+BETA2*X2+BETA3*X3+BETA4*X1*X2+BETA5*X1*X3+
929        1        BETA6*X2*X3+BETA7*X1*X2*X3
930               WRITE (53,875)X1*100.,X2*100.,X3*100.,Y    ! OUTPUT TO 9876
931               X1=1.0
932               X2=0.0
933               X3=0.0
934               Y=BETA1*X1+BETA2*X2+BETA3*X3+BETA4*X1*X2+BETA5*X1*X3+
935        1        BETA6*X2*X3+BETA7*X1*X2*X3
936               WRITE (53,875)X1*100.,X2*100.,X3*100.,Y    ! OUTPUT TO 9876
937               WRITE (53,891)                             ! OUTPUT TO 9876
938               PAGE=PAGE+1
```

```
939               IF (PLOT.NE.1) GOTO 740
940               WRITE (53,876)                                  ! OUTPUT TO 9876
941 ***     PLOT TRIANGLE ON CRT
942               G1=10.
943               G2=400.
944               Y_INCR=G2*(SQRT(3.0)/2)/10.
945               DO 645 I1=0,10
946                  F=I1
947                  XB(I1)=INT(G1+(Y_INCR*F)/(SQRT(3.0)/2))
948                  YB(I1)=INT(G1)
949                  XL(I1)=INT(G1+(Y_INCR*F)/(SQRT(3.0)/1))
950                  YL(I1)=INT(G1+(Y_INCR*F))
951                  XR(I1)=INT(G1+(Y_INCR*10+Y_INCR*F)/(SQRT(3.0)/1))
952                  YR(I1)=INT(G1+(Y_INCR*(10-I1)))
953  645          CONTINUE
954 C         CLEAR SCREEN AND INITIALIZE 2648 GRAPHICS
955               WRITE (1,877) ESC,ESC,ESC,ESC
956               LM1=10/2
957               DO 650 N1=0,5                    ! DRAW TRIANGLE ON THE CRT
958                  WRITE (1,878) ESC,XL(N1),YL(N1)
959                  WRITE (1,880) ESC,XB(N1),YB(N1),ESC,XR(N1),YR(N1)
960                  IF (N1.LT.LM1) THEN
961                     N2=10-N1
962                     WRITE (1,880) ESC,XL(N2),YL(N2),ESC,XB(N2),YB(N2),
963       1             ESC,XR(N2),YR(N2)
964                  ENDIF
965                  WRITE (1,880) ESC,XL(N1),YL(N1)
966  650          CONTINUE
967               WRITE (1,879) ESC,ESC,ESC,ESC  ! LABLE THE TRIANGLE
968 *
969 ******** PLOT LINES OF RESOLUTION
970 *
971               Y=RESWANT
972               MARK=1
973               GOTO 700
974  655          Y=0
975               MARK=2
976               GOTO 700
977  660          Y=-RESWANT
978               MARK=3
979 *********  CALCULATES PREDICTED RESOLUTION VALUES
980  700          N=1
981               M=1
982               DO 715 X=0,100
983                  X1=X/100
984                  C1=BETA3+(BETA1-BETA3+BETA5-BETA5*X1)*X1
985                  C2=BETA2-BETA3+BETA6+(BETA4-BETA5-BETA6+BETA7-
986       1             BETA7*X1)*X1
987                  C3=0-BETA6-BETA7*X1
988                  A=C3
989                  B=C2
990                  C=C1-Y
991                  D=B*B-4*A*C
992                  IF (D.LT.0) GOTO 715
993                  S=SQRT(D)
994                  R1=(0-B+S)/(2*A)
995                  R2=(0-B-S)/(2*A)
996  705             IF (R1.LT.0.OR.R1.GT.1) GOTO 710
997                  Q1=X1+R1
998                  IF (Q1.GT.1) GOTO 710
999                  X2=1-Q1
```

```
1000                X3=R1
1001                XARRAY(N)=G1+(X3+X1/2)*G2
1002                YARRAY(N)=G1+X1*G2*SQRT(3.0)/2
1003                N=N+1
1004  710           IF (R2.LT.0.OR.R2.GT.1) GOTO 715
1005                Q2=X1+R2
1006                IF (Q2.GT.1) GOTO 715
1007                X2=1-Q2
1008                X3=R2
1009                PARRAY(M)=G1+(X3+X1/2)*G2
1010                QARRAY(M)=G1+(X1*G2*SQRT(3.0)/2)
1011                M=M+1
1012  715           CONTINUE
1013              IF (N.LT.3) GOTO 725
1014              XMOVE=XARRAY(1)
1015              YMOVE=YARRAY(1)
1016 ***       DRAW RESOLUTION LINES ONTO TRIANGLE
1017              DO 720 I8=2,N-1
1018                 XDRAW=XARRAY(I8)
1019                 YDRAW=YARRAY(I8)
1020 C             DRAW RESOLUTION LINES
1021                 WRITE (1,878) ESC,XMOVE,YMOVE
1022                 WRITE (1,880) ESC,XDRAW,YDRAW
1023                 XMOVE=XDRAW
1024                 YMOVE=YDRAW
1025  720           CONTINUE
1026              WRITE (1,881) ESC,Y
1027  725         WRITE (1,882) ESC
1028              IF (M.LT.3) GOTO (655,660,735) MARK
1029              XMOVE=PARRAY(1)
1030              YMOVE=QARRAY(1)
1031              DO 730 I8=2,M-1
1032                 XDRAW=PARRAY(I8)
1033                 YDRAW=QARRAY(I8)
1034 C             DRAW RESOLUTION LINES
1035                 WRITE (1,878) ESC,XMOVE,YMOVE
1036                 WRITE (1,880) ESC,XDRAW,YDRAW
1037                 XMOVE=XDRAW
1038                 YMOVE=YDRAW
1039  730           CONTINUE
1040              WRITE (1,881) ESC,Y    ! PRINT RESOLUTION ON TRIANGLE
1041              WRITE (1,882) ESC      ! TURN OFF GRAPHICS TEXT
1042              GOTO (655,660,735) MARK
1043  735         WRITE (1,883) ESC,ESC  ! TRANSFER GRAPHICS TO 9876 VIA HPIB
1044              CALL WAIT (37,2)       ! WAIT FOR RASTER DUMP TO FINISH
1045              WRITE (1,873) ESC,ESC,ESC,ESC ! FORM FEED 9876
1046              PAGE=1
1047              IF (PLOT.EQ.1) GOTO 745
1048  740         WRITE (53,884) PEAKNAME(I)(:13),PEAKNAME(J),RESWANT
1049  745       CONTINUE
1050  750   CONTINUE
1051        WRITE (1,885)
1052        WRITE (1,886) ESC          ! TURN OFF GRAPHICS DISPLAY
1053        READ (1,890) QUEST         ! DUMMY TO TAKE "S" FROM PRINTER
1054        WRITE (1,889) ESC,ESC      ! ERASE "S" FROM SCREEN
1055        READ  1,890) QUEST
1056        IF (QUEST.NE.'Y') RETURN
1057        GOTO 600
1058  870   FORMAT (//,'PEAK PAIRS ALWAYS RESOLVED GREATER THAN ',F5.2,
1059       1' WILL BE IGNORED!')
1060  871   FORMAT (A1,'H',A1,'J',//,'FOR PEAK PAIR  ',A15,'- ',A15)
```

```
1061   872  FORMAT (//,'CHECKING FOR RESOLUTION OF ',F5.2)
1062   873  FORMAT(A1,'Y',A1,'U',A1,'Z',A1,'&p3s5dB')
1063   874  FORMAT(//,T15,'FOR PEAK PAIR  ',A15,'-  ',A15,//,T25,'BETA ',
1064       1'COEFFICIENTS (1-7)',/,T10,7F8.3,//,T23,'MEOH',T37,'ACN',T52,
1065       1'THF',T65,'RESOLUTION')
1066   875  FORMAT(T22,I4,'%',T36,I4,'%',T51,I4,'%',T61,F12.3)
1067   876  FORMAT (//,' ',//)
1068   877  FORMAT (A1,'H',A1,'J',A1,'*m2a 0,0 j1bz',A1,'*dach1ntz')
1069   878  FORMAT (A1,'*pah',2I4,'Z')
1070   879  FORMAT(A1,'*d 0,0 okSTHF',A1,'*d 400,0 OACN',A1,'*d 230,350 '
1071       1'OMeOH',A1,'*d1T')
1072   880  FORMAT (A1,'*pbh',2I4,'Z')
1073   881  FORMAT (A1,'*dsZ',F5.2)
1074   882  FORMAT (A1,'*dtZ')
1075   883  FORMAT (A1,'&p5D',A1,'&p5u0C')
1076   884  FORMAT ('PEAK PAIR  ',R15,'- ',A15,' IS ALWAYS RESOLVED ',
1077       1'BETTER THAN ',F5.2,//)
1078   885  FORMAT (/,'DO YOU WANT TO PLOT A DIFFERENT RESOLUTION? _')
1079   886  FORMAT(A1,'*dD')
1080   887  FORMAT(A1,'H',A1,'J')
1081   888  FORMAT (T30,'HPLC OPTIMIZATION',/,T23,15A2,//,T32,
1082       1'DATA ANALYSIS',/,T20,'COLUMN :',A16,T45,'SAMPLE :',A16,//,
1083       1T2,//,A1,'H',A1,'&p3s5dF')
1084   889  FORMAT (A1,'A',A1,'J')
1085   890  FORMAT (A1)
1086   891  FORMAT (T17,'-------------------------------------------------',
1087       1'----------')
1088        END
```

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